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```
REMARK coordinates from restrained individual B-factor refinement
REMARK refinement resolution: 500.0 - 1.65 Å
REMARK starting r= 0.2072 free_r= 0.2361
REMARK final r= 0.2072 free_r= 0.2361
REMARK B rmsd for bonded mainchain atoms= 1.427 target= 1.5
REMARK B rmsd for bonded sidechain atoms= 2.420 target= 2.0
REMARK B rmsd for angle mainchain atoms= 2.189 target= 2.0
REMARK B rmsd for angle sidechain atoms= 3.637 target= 2.5
REMARK rweight= 0.1000 (with w= 0.987736)
REMARK target= mlf steps= 30
REMARK sg= P1 a= 41.23 b= 65.22 c= 73.38 alpha= 73.11 beta= 85.58 gamma= 85.8
REMARK parameter file 1 : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2 : CNS_TOPPAR:water_rep.param
REMARK molecular structure file: amy.mtf
REMARK input coordinates: amy.pdb
REMARK reflection file= amy.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.65
REMARK initial B-factor correction applied to fobs :
REMARK B11= -3.662 B22= 2.485 B33= 1.177
REMARK B12= 2.042 B13= 2.748 B23= -0.502
REMARK B-factor correction applied to coordinate array B: 0.012
REMARK bulk solvent: density level= 0.36444 e/Å³, B-factor= 46.0136 Å²
REMARK reflections with |Fobs|/sigma F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range: 87646 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0): 2854 ( 3.3 % )
REMARK number of reflections rejected: 0 ( 0.0 % )
REMARK total number of reflections used: 84792 ( 96.7 % )
REMARK number of reflections in working set: 80566 ( 91.9 % )
REMARK number of reflections in test set: 4226 ( 4.8 % )
CRYST1 41.230 65.220 73.380 73.11 85.58 85.80 P 1
REMARK FILENAME="/work/olieric/db/db2-5 P1/cns/bindividual.pdb"
REMARK DATE: 31-Mar-03 11:57:01 created by user: olieric
REMARK VERSION: 1.1
ATOM 1 CB MET A 1 -14.276 -31.220 16.788 1.00 17.29 A
ATOM 2 CG MET A 1 -13.562 -30.976 15.453 1.00 19.06 A
ATOM 3 SD MET A 1 -13.791 -29.325 14.750 1.00 20.01 A
ATOM 4 CE MET A 1 -12.595 -28.385 15.663 1.00 20.04 A
ATOM 5 C MET A 1 -12.346 -32.264 17.931 1.00 17.38 A
ATOM 6 O MET A 1 -12.094 -31.451 18.823 1.00 18.05 A
ATOM 7 N MET A 1 -14.641 -32.810 18.672 1.00 17.69 A
ATOM 8 CA MET A 1 -13.789 -32.489 17.479 1.00 17.26 A
ATOM 9 N LYS A 2 -11.404 -32.959 17.305 1.00 16.63 A
ATOM 10 CA LYS A 2 -9.991 -32.827 17.687 1.00 17.10 A
ATOM 11 CB LYS A 2 -9.686 -33.813 18.819 1.00 20.78 A
ATOM 12 CG LYS A 2 -8.255 -33.915 19.217 1.00 24.62 A
ATOM 13 CD LYS A 2 -8.095 -34.972 20.295 1.00 28.83 A
ATOM 14 CE LYS A 2 -6.710 -34.905 20.918 1.00 31.65 A
ATOM 15 NZ LYS A 2 -6.617 -35.825 22.100 1.00 33.43 A
ATOM 16 C LYS A 2 -9.119 -33.168 16.483 1.00 17.18 A
ATOM 17 O LYS A 2 -9.455 -34.064 15.706 1.00 14.51 A
ATOM 18 N PHE A 3 -8.034 -32.423 16.284 1.00 14.64 A
ATOM 19 CA PHE A 3 -7.135 -32.762 15.187 1.00 14.50 A
ATOM 20 CB PHE A 3 -7.652 -32.265 13.810 1.00 16.07 A
ATOM 21 CG PHE A 3 -7.818 -30.761 13.686 1.00 15.16 A
ATOM 22 CD1 PHE A 3 -9.067 -30.157 13.880 1.00 15.68 A
ATOM 23 CD2 PHE A 3 -6.737 -29.955 13.299 1.00 12.43 A
ATOM 24 CE1 PHE A 3 -9.233 -28.776 13.690 1.00 15.69 A
ATOM 25 CE2 PHE A 3 -6.888 -28.598 13.109 1.00 15.35 A
ATOM 26 C PHE A 3 -8.163 -27.996 13.313 1.00 14.58 A
ATOM 27 O PHE A 3 -5.783 -32.146 15.480 1.00 15.40 A
ATOM 28 O PHE A 3 -5.685 -31.234 16.283 1.00 14.89 A
ATOM 29 N THR A 4 -4.732 -32.697 14.884 1.00 13.77 A
ATOM 30 CA THR A 4 -3.407 -32.124 15.046 1.00 15.62 A
ATOM 31 CB THR A 4 -2.486 -32.956 15.948 1.00 17.56 A
ATOM 32 CG1 THR A 4 -3.030 -32.988 17.274 1.00 18.68 A
ATOM 33 CG2 THR A 4 -1.084 -32.288 16.013 1.00 18.01 A
ATOM 34 C THR A 4 -2.846 -32.111 13.645 1.00 15.42 A
ATOM 35 O THR A 4 -2.880 -33.120 12.942 1.00 17.97 A
ATOM 36 N VAL A 5 -2.317 -30.970 13.238 1.00 16.55 A
ATOM 37 CA VAL A 5 -1.804 -30.886 11.883 1.00 16.64 A
ATOM 38 CB VAL A 5 -2.948 -30.508 10.930 1.00 18.41 A
ATOM 39 CG1 VAL A 5 -3.416 -29.040 11.181 1.00 18.38 A
ATOM 40 CG2 VAL A 5 -2.514 -30.773 9.468 1.00 19.99 A
ATOM 41 C VAL A 5 -0.679 -29.886 11.773 1.00 17.93 A
ATOM 42 O VAL A 5 -0.559 -28.960 12.592 1.00 16.18 A
ATOM 43 N GLU A 6 0.166 -30.070 10.765 1.00 16.71 A
ATOM 44 CA GLU A 6 1.253 -29.120 10.579 1.00 18.01 A
ATOM 45 CB GLU A 6 2.218 -29.605 9.499 1.00 19.85 A
ATOM 46 CG GLU A 6 3.012 -30.850 9.875 1.00 24.39 A
ATOM 47 CD GLU A 6 3.999 -31.273 8.780 1.00 30.54 A
ATOM 48 OE1 GLU A 6 4.475 -30.396 8.006 1.00 30.19 A
ATOM 49 OE2 GLU A 6 4.317 -32.484 8.709 1.00 31.65 A
ATOM 50 C GLU A 6 0.734 -27.751 10.164 1.00 17.50 A
ATOM 51 O GLU A 6 -0.166 -27.642 9.334 1.00 17.39 A
ATOM 52 N ARG A 7 1.337 -26.703 10.717 1.00 15.98 A
ATOM 53 CA ARG A 7 0.975 -25.341 10.359 1.00 16.73 A
ATOM 54 CB ARG A 7 1.939 -24.375 11.051 1.00 16.92 A
ATOM 55 CG ARG A 7 1.902 -22.950 10.542 1.00 15.16 A
ATOM 56 CD ARG A 7 3.010 -22.130 11.223 1.00 15.81 A
ATOM 57 NE ARG A 7 3.117 -20.745 10.778 1.00 16.48 A
ATOM 58 CZ ARG A 7 3.906 -20.342 9.787 1.00 19.48 A
ATOM 59 NH1 ARG A 7 4.650 -21.243 9.135 1.00 19.10 A
ATOM 60 NH2 ARG A 7 3.953 -19.063 9.445 1.00 19.15 A
ATOM 61 C ARG A 7 1.077 -25.168 8.842 1.00 19.33 A
ATOM 62 O ARG A 7 0.232 -24.536 8.201 1.00 20.23 A
ATOM 63 N GLU A 8 2.116 -25.777 8.284 1.00 20.57 A
ATOM 64 CA GLU A 8 2.392 -25.680 6.869 1.00 23.30 A
ATOM 65 CB GLU A 8 3.669 -26.474 6.585 1.00 25.23 A
```

BEST AVAILABLE COPY

Figure 1 (1)

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ATOM	66	CG	GLU	A	8	4.958	-25.909	7.259	1.00	29.45	A
ATOM	67	CD	GLU	A	8	4.840	-25.478	8.733	1.00	28.90	A
ATOM	68	OE1	GLU	A	8	4.512	-26.346	9.633	1.00	28.78	A
ATOM	69	OE2	GLU	A	8	5.119	-24.257	8.986	1.00	23.71	A
ATOM	70	C	GLU	A	8	1.213	-26.154	6.007	1.00	22.79	A
ATOM	71	O	HIS	A	9	0.997	-25.624	4.913	1.00	24.80	A
ATOM	72	N	HIS	A	9	0.433	-27.108	6.514	1.00	21.38	A
ATOM	73	CA	HIS	A	9	-0.711	-27.627	5.748	1.00	21.73	A
ATOM	74	CB	HIS	A	9	-1.034	-29.064	6.157	1.00	23.42	A
ATOM	75	CG	HIS	A	9	0.111	-30.021	6.010	1.00	27.55	A
ATOM	76	CD2	HIS	A	9	1.279	-29.926	5.335	1.00	29.37	A
ATOM	77	ND1	HIS	A	9	0.136	-31.242	6.644	1.00	27.98	A
ATOM	78	CE1	HIS	A	9	1.273	-31.856	6.376	1.00	28.44	A
ATOM	79	NE2	HIS	A	9	1.986	-31.080	5.583	1.00	30.06	A
ATOM	80	C	HIS	A	9	-1.974	-26.796	5.903	1.00	22.06	A
ATOM	81	O	HIS	A	9	-2.916	-26.941	5.113	1.00	20.93	A
ATOM	82	N	LEU	A	10	-2.007	-25.930	6.909	1.00	20.66	A
ATOM	83	CA	LEU	A	10	-3.169	-25.074	7.155	1.00	21.35	A
ATOM	84	CB	LEU	A	10	-3.366	-24.857	8.655	1.00	21.25	A
ATOM	85	CG	LEU	A	10	-4.041	-25.917	9.494	1.00	22.14	A
ATOM	86	CD1	LEU	A	10	-4.016	-25.491	10.958	1.00	22.44	A
ATOM	87	CD2	LEU	A	10	-5.499	-26.105	9.002	1.00	19.68	A
ATOM	88	C	LEU	A	10	-3.135	-23.695	6.547	1.00	22.26	A
ATOM	89	O	LEU	A	10	-4.182	-23.091	6.321	1.00	24.22	A
ATOM	90	N	LEU	A	11	-1.935	-23.173	6.349	1.00	22.98	A
ATOM	91	CA	LEU	A	11	-1.731	-21.819	5.853	1.00	25.99	A
ATOM	92	CB	LEU	A	11	-0.223	-21.587	5.647	1.00	27.18	A
ATOM	93	CG	LEU	A	11	0.489	-20.748	6.712	1.00	31.58	A
ATOM	94	CD1	LEU	A	11	-0.093	-20.987	8.066	1.00	31.86	A
ATOM	95	CD2	LEU	A	11	1.991	-21.058	6.673	1.00	31.87	A
ATOM	96	C	LEU	A	11	-2.497	-21.417	4.602	1.00	24.67	A
ATOM	97	O	LEU	A	11	-3.300	-20.487	4.638	1.00	24.80	A
ATOM	98	N	LYS	A	12	-2.270	-22.122	3.507	1.00	24.14	A
ATOM	99	CA	LYS	A	12	-2.949	-21.784	2.263	1.00	25.70	A
ATOM	100	CB	LYS	A	12	-2.393	-22.627	1.102	1.00	28.62	A
ATOM	101	CG	LYS	A	12	-2.758	-22.084	-0.282	1.00	33.62	A
ATOM	102	CD	LYS	A	12	-2.196	-22.974	-1.407	1.00	36.68	A
ATOM	103	CE	LYS	A	12	-3.036	-24.242	-1.643	1.00	39.26	A
ATOM	104	NZ	LYS	A	12	-3.304	-25.093	-0.433	1.00	38.28	A
ATOM	105	C	LYS	A	12	-4.458	-21.963	2.397	1.00	22.87	A
ATOM	106	O	LYS	A	12	-5.233	-21.072	2.031	1.00	24.13	A
ATOM	107	N	PRO	A	13	-4.906	-23.118	2.922	1.00	21.49	A
ATOM	108	CD	PRO	A	13	-4.218	-24.387	3.212	1.00	21.35	A
ATOM	109	CA	PRO	A	13	-6.359	-23.257	3.052	1.00	21.39	A
ATOM	110	CB	PRO	A	13	-6.521	-24.589	3.774	1.00	20.96	A
ATOM	111	CG	PRO	A	13	-5.337	-25.379	3.227	1.00	21.10	A
ATOM	112	C	PRO	A	13	-6.972	-22.103	3.836	1.00	20.93	A
ATOM	113	O	PRO	A	13	-7.985	-21.545	3.431	1.00	21.33	A
ATOM	114	N	LEU	A	14	-6.369	-21.735	4.967	1.00	21.72	A
ATOM	115	CA	LEU	A	14	-6.920	-20.646	5.762	1.00	22.99	A
ATOM	116	CB	LEU	A	14	-6.111	-20.432	7.048	1.00	22.66	A
ATOM	117	CG	LEU	A	14	-6.506	-21.332	8.208	1.00	19.80	A
ATOM	118	CD1	LEU	A	14	-5.520	-21.068	9.351	1.00	19.78	A
ATOM	119	CD2	LEU	A	14	-7.951	-21.053	8.667	1.00	19.15	A
ATOM	120	C	LEU	A	14	-6.992	-19.318	5.041	1.00	26.19	A
ATOM	121	O	LEU	A	14	-7.964	-18.577	5.189	1.00	27.05	A
ATOM	122	N	GLN	A	15	-5.947	-18.995	4.297	1.00	27.38	A
ATOM	123	CA	GLN	A	15	-5.935	-17.742	3.574	1.00	31.46	A
ATOM	124	CB	GLN	A	15	-4.608	-17.570	2.842	1.00	33.84	A
ATOM	125	CG	GLN	A	15	-4.472	-16.213	2.182	1.00	38.53	A
ATOM	126	CD	GLN	A	15	-3.117	-16.025	1.545	1.00	41.36	A
ATOM	127	OE1	GLN	A	15	-2.080	-16.062	2.223	1.00	42.71	A
ATOM	128	NE2	GLN	A	15	-3.109	-15.827	0.230	1.00	43.79	A
ATOM	129	C	GLN	A	15	-7.081	-17.731	2.568	1.00	32.51	A
ATOM	130	O	GLN	A	15	-7.813	-16.741	2.440	1.00	32.62	A
ATOM	131	N	GLN	A	16	-7.250	-18.852	1.878	1.00	32.52	A
ATOM	132	CA	GLN	A	16	-8.284	-18.960	0.862	1.00	33.60	A
ATOM	133	CB	GLN	A	16	-8.191	-20.314	0.161	1.00	34.74	A
ATOM	134	CG	GLN	A	16	-9.193	-20.486	-0.970	1.00	38.72	A
ATOM	135	CD	GLN	A	16	-8.630	-20.088	-2.328	1.00	41.86	A
ATOM	136	OE1	GLN	A	16	-8.139	-18.960	-2.519	1.00	42.92	A
ATOM	137	NE2	GLN	A	16	-8.701	-21.018	-3.286	1.00	41.57	A
ATOM	138	C	GLN	A	16	-9.698	-18.767	1.398	1.00	32.72	A
ATOM	139	O	GLN	A	16	-10.502	-18.042	0.808	1.00	33.73	A
ATOM	140	N	VAL	A	17	-10.018	-19.396	2.521	1.00	31.34	A
ATOM	141	CA	VAL	A	17	-11.371	-19.262	3.041	1.00	32.67	A
ATOM	142	CB	VAL	A	17	-11.801	-20.516	3.822	1.00	29.85	A
ATOM	143	CG1	VAL	A	17	-11.679	-21.733	2.928	1.00	28.35	A
ATOM	144	CG2	VAL	A	17	-10.948	-20.683	5.063	1.00	29.58	A
ATOM	145	C	VAL	A	17	-11.608	-18.045	3.917	1.00	35.48	A
ATOM	146	O	VAL	A	17	-12.757	-17.663	4.130	1.00	34.98	A
ATOM	147	N	SER	A	18	-10.539	-17.448	4.431	1.00	39.01	A
ATOM	148	CA	SER	A	18	-10.672	-16.274	5.294	1.00	43.39	A
ATOM	149	CB	SER	A	18	-9.520	-16.308	6.292	1.00	43.24	A
ATOM	150	CG	SER	A	18	-9.475	-17.366	7.099	1.00	44.08	A
ATOM	151	C	SER	A	18	-10.695	-14.590	4.477	1.00	46.76	A
ATOM	152	O	SER	A	18	-11.095	-13.932	4.982	1.00	46.88	A
ATOM	153	N	GLY	A	19	-10.266	-15.096	3.221	1.00	50.03	A
ATOM	154	CA	GLY	A	19	-10.221	-13.953	2.322	1.00	54.68	A
ATOM	155	C	GLY	A	19	-11.387	-12.985	2.438	1.00	57.76	A
ATOM	156	O	GLY	A	19	-11.234	-11.899	3.011	1.00	58.12	A
ATOM	157	N	PRO	A	20	-12.566	-13.333	1.893	1.00	60.08	A
ATOM	158	CB	PRO	A	20	-12.947	-14.603	1.250	1.00	60.71	A
ATOM	159	CA	PRO	A	20	-13.713	-12.425	1.989	1.00	62.25	A
ATOM	160	CG	PRO	A	20	-14.831	-13.208	1.289	1.00	62.05	A
ATOM	161	C	PRO	A	20	-14.434	-14.648	1.497	1.00	61.28	A
ATOM	162	O	PRO	A	20	-14.040	-12.092	3.450	1.00	64.35	A
ATOM	163	N	LEU	A	21	-14.838	-12.786	4.088	1.00	64.86	A
ATOM	164	C	LEU	A	21	-13.420	-11.032	3.976	1.00	66.50	A
ATOM	165	CA	LEU	A	21	-13.636	-10.631	5.368	1.00	68.70	A

Figure 1 (continued 2)

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ATOM	166	CB	LEU	A	21	-13.417	-11.842	6.292	1.00	68.85	A
ATOM	167	CG	LEU	A	21	-13.658	-11.701	7.797	1.00	69.20	A
ATOM	168	CD1	LEU	A	21	-15.091	-11.257	8.058	1.00	69.44	A
ATOM	169	CD2	LEU	A	21	-13.383	-13.037	8.473	1.00	69.17	A
ATOM	170	O	LEU	A	21	-12.744	-9.468	5.837	1.00	69.92	A
ATOM	171	O	LEU	A	21	-11.823	-9.033	5.133	1.00	70.14	A
ATOM	172	N	GLY	A	22	-13.029	-8.981	7.043	1.00	70.90	A
ATOM	173	CA	GLY	A	22	-12.270	-7.883	7.608	1.00	72.13	A
ATOM	174	C	GLY	A	22	-13.141	-6.650	7.685	1.00	73.06	A
ATOM	175	O	GLY	A	22	-13.445	-6.156	8.773	1.00	73.37	A
ATOM	176	N	GLY	A	23	-13.556	-6.165	6.518	1.00	73.72	A
ATOM	177	CA	GLY	A	23	-14.395	-4.982	6.447	1.00	74.72	A
ATOM	178	C	GLY	A	23	-15.796	-5.167	7.006	1.00	74.24	A
ATOM	179	O	GLY	A	23	-16.645	-5.826	6.394	1.00	74.63	A
ATOM	180	N	ARG	A	24	-16.028	-4.573	8.176	1.00	74.77	A
ATOM	181	CA	ARG	A	24	-17.315	-4.624	8.865	1.00	74.14	A
ATOM	182	CB	ARG	A	24	-18.178	-3.428	8.440	1.00	75.43	A
ATOM	183	CG	ARG	A	24	-19.494	-3.302	9.198	1.00	77.04	A
ATOM	184	CD	ARG	A	24	-20.297	-2.119	8.683	1.00	78.78	A
ATOM	185	NE	ARG	A	24	-21.576	-1.972	9.373	1.00	80.11	A
ATOM	186	CZ	ARG	A	24	-22.483	-1.049	9.068	1.00	80.78	A
ATOM	187	NH1	ARG	A	24	-22.251	-0.188	8.084	1.00	81.08	A
ATOM	188	NH2	ARG	A	24	-23.623	-0.988	9.744	1.00	81.03	A
ATOM	189	C	ARG	A	24	-18.102	-5.919	8.655	1.00	72.74	A
ATOM	190	O	ARG	A	24	-19.099	-5.940	7.932	1.00	73.15	A
ATOM	191	N	PRO	A	25	-17.659	-7.021	9.280	1.00	71.00	A
ATOM	192	CA	PRO	A	25	-16.401	-7.195	10.026	1.00	70.86	A
ATOM	193	CB	PRO	A	25	-18.367	-8.297	9.129	1.00	69.14	A
ATOM	194	C	PRO	A	25	-17.526	-9.256	9.967	1.00	69.82	A
ATOM	195	CG	PRO	A	25	-16.138	-8.670	9.855	1.00	70.46	A
ATOM	196	O	PRO	A	25	-19.787	-8.152	9.673	1.00	67.21	A
ATOM	197	N	THR	A	26	-19.964	-7.852	10.852	1.00	67.34	A
ATOM	198	CA	THR	A	26	-20.794	-8.352	8.825	1.00	64.60	A
ATOM	199	CB	THR	A	26	-22.184	-8.218	9.265	1.00	61.62	A
ATOM	200	CG	THR	A	26	-23.179	-8.457	8.100	1.00	62.41	A
ATOM	201	OG1	THR	A	26	-22.829	-7.625	6.986	1.00	62.97	A
ATOM	202	OG2	THR	A	26	-24.598	-9.102	8.535	1.00	62.89	A
ATOM	203	C	THR	A	26	-22.487	-9.199	10.399	1.00	58.62	A
ATOM	204	O	THR	A	26	-21.891	-9.105	11.474	1.00	58.71	A
ATOM	205	N	LEU	A	27	-23.413	-10.128	10.167	1.00	54.49	A
ATOM	206	CA	LEU	A	27	-23.766	-11.123	11.177	1.00	49.96	A
ATOM	207	CB	LEU	A	27	-24.522	-12.298	10.546	1.00	50.45	A
ATOM	208	CG	LEU	A	27	-25.845	-12.037	9.828	1.00	50.99	A
ATOM	209	CD1	LEU	A	27	-25.611	-11.122	8.637	1.00	51.87	A
ATOM	210	CD2	LEU	A	27	-26.450	-13.356	9.361	1.00	51.62	A
ATOM	211	O	LEU	A	27	-22.461	-11.627	11.791	1.00	46.57	A
ATOM	212	N	PRO	A	28	-21.498	-11.909	11.076	1.00	45.78	A
ATOM	213	CA	PRO	A	28	-22.406	-11.734	13.125	1.00	42.86	A
ATOM	214	CB	PRO	A	28	-23.458	-11.471	14.125	1.00	42.50	A
ATOM	215	C	PRO	A	28	-21.179	-12.207	13.770	1.00	39.77	A
ATOM	216	CG	PRO	A	28	-21.586	-12.325	15.243	1.00	40.55	A
ATOM	217	O	PRO	A	28	-22.641	-11.263	15.384	1.00	41.64	A
ATOM	218	N	ILE	A	29	-20.704	-13.536	13.197	1.00	36.67	A
ATOM	219	CA	ILE	A	29	-19.502	-13.737	12.978	1.00	35.24	A
ATOM	220	CB	ILE	A	29	-21.659	-14.434	12.964	1.00	33.25	A
ATOM	221	CG	ILE	A	29	-21.389	-15.764	12.440	1.00	31.49	A
ATOM	222	OG1	ILE	A	29	-22.725	-16.518	12.190	1.00	32.34	A
ATOM	223	OG2	ILE	A	29	-23.443	-15.893	11.009	1.00	32.60	A
ATOM	224	C	ILE	A	29	-22.486	-18.006	11.925	1.00	33.89	A
ATOM	225	O	ILE	A	29	-22.008	-18.774	13.115	1.00	33.09	A
ATOM	226	N	LEU	A	30	-20.600	-15.694	11.137	1.00	29.03	A
ATOM	227	CA	LEU	A	30	-19.779	-16.569	10.860	1.00	27.06	A
ATOM	228	CB	LEU	A	30	-20.810	-14.645	10.352	1.00	27.42	A
ATOM	229	C	LEU	A	30	-20.124	-14.555	9.059	1.00	26.34	A
ATOM	230	CG	LEU	A	30	-20.837	-13.539	8.153	1.00	27.73	A
ATOM	231	CD1	LEU	A	30	-22.319	-13.856	7.930	1.00	29.16	A
ATOM	232	CD2	LEU	A	30	-22.901	-12.767	7.025	1.00	29.49	A
ATOM	233	O	LEU	A	30	-22.528	-15.249	7.312	1.00	28.59	A
ATOM	234	N	LEU	A	30	-18.640	-14.238	9.154	1.00	24.62	A
ATOM	235	CA	GLY	A	31	-17.910	-14.362	8.168	1.00	24.88	A
ATOM	236	C	GLY	A	31	-18.190	-13.860	10.350	1.00	21.78	A
ATOM	237	O	GLY	A	31	-16.789	-13.553	10.548	1.00	21.58	A
ATOM	238	N	GLY	A	31	-16.069	-14.788	11.093	1.00	19.65	A
ATOM	239	CA	ASN	A	32	-14.889	-14.720	11.414	1.00	21.22	A
ATOM	240	CB	ASN	A	32	-16.784	-15.895	11.182	1.00	19.33	A
ATOM	241	CG	ASN	A	32	-16.221	-17.164	11.678	1.00	17.81	A
ATOM	242	OD1	ASN	A	32	-17.174	-17.859	12.668	1.00	18.05	A
ATOM	243	OD2	ASN	A	32	-17.079	-17.275	14.077	1.00	14.39	A
ATOM	244	N	ASN	A	32	-16.566	-16.193	14.234	1.00	18.82	A
ATOM	245	C	ASN	A	32	-17.541	-18.018	15.082	1.00	16.05	A
ATOM	246	O	ASN	A	32	-16.006	-18.109	10.524	1.00	19.88	A
ATOM	247	N	LEU	A	33	-16.554	-17.930	9.426	1.00	20.74	A
ATOM	248	CA	LEU	A	33	-15.178	-19.116	10.781	1.00	19.03	A
ATOM	249	CB	LEU	A	33	-14.924	-20.155	9.804	1.00	18.58	A
ATOM	250	CG	LEU	A	33	-13.435	-20.435	9.671	1.00	20.53	A
ATOM	251	CD1	LEU	A	33	-12.569	-19.411	8.996	1.00	22.72	A
ATOM	252	CD2	LEU	A	33	-11.137	-19.964	8.958	1.00	25.09	A
ATOM	253	O	LEU	A	33	-13.107	-19.134	7.606	1.00	25.02	A
ATOM	254	N	LEU	A	34	-15.530	-21.398	10.365	1.00	18.12	A
ATOM	255	CA	LEU	A	34	-15.430	-21.648	11.576	1.00	17.01	A
ATOM	256	CB	LEU	A	34	-16.184	-22.179	9.513	1.00	15.99	A
ATOM	257	CG	LEU	A	34	-16.730	-23.433	9.951	1.00	16.00	A
ATOM	258	OD1	LEU	A	34	-17.914	-23.864	9.073	1.00	18.73	A
ATOM	259	OD2	LEU	A	34	-18.416	-25.301	9.197	1.00	17.56	A
ATOM	260	C	LEU	A	34	-18.968	-25.610	10.583	1.00	20.61	A
ATOM	261	O	LEU	A	34	-19.527	-25.480	8.138	1.00	20.63	A
ATOM	262	N	LEU	A	34	-15.618	-24.467	9.807	1.00	17.87	A
ATOM	263	CA	LEU	A	35	-15.009	-24.561	8.725	1.00	18.24	A
ATOM	264	CB	LEU	A	35	-15.335	-25.196	10.893	1.00	16.38	A
ATOM	265	CG	LEU	A	35	-14.346	-26.290	10.903	1.00	16.62	A

Figure 1 (continued 3)

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ATOM	266	CB	LEU	A	35	-13.301	-26.110	12.029	1.00	16.55	A
ATOM	267	CG	LEU	A	35	-12.328	-24.919	11.927	1.00	20.44	A
ATOM	268	CD1	LEU	A	35	-13.026	-23.564	11.887	1.00	26.52	A
ATOM	269	CD2	LEU	A	35	-11.438	-24.958	13.149	1.00	22.52	A
ATOM	270	C	LEU	A	35	-15.083	-27.609	11.117	1.00	16.64	A
ATOM	271	O	LEU	A	35	-15.859	-27.763	12.066	1.00	15.83	A
ATOM	272	N	GLN	A	36	-14.857	-28.572	10.227	1.00	15.28	A
ATOM	273	CA	GLN	A	36	-15.520	-29.866	10.344	1.00	15.61	A
ATOM	274	CB	GLN	A	36	-16.596	-29.997	9.238	1.00	17.87	A
ATOM	275	CG	GLN	A	36	-17.676	-28.913	9.217	1.00	23.26	A
ATOM	276	CD	GLN	A	36	-18.504	-28.948	7.921	1.00	27.12	A
ATOM	277	OE1	GLN	A	36	-19.714	-29.221	7.953	1.00	31.11	A
ATOM	278	NE2	GLN	A	36	-17.850	-28.676	6.775	1.00	26.03	A
ATOM	279	C	GLN	A	36	-14.507	-30.996	10.156	1.00	16.00	A
ATOM	280	O	GLN	A	36	-13.767	-30.971	9.177	1.00	17.23	A
ATOM	281	N	VAL	A	37	-14.461	-31.947	11.097	1.00	14.69	A
ATOM	282	CA	VAL	A	37	-13.594	-33.123	10.959	1.00	15.63	A
ATOM	283	CB	VAL	A	37	-12.796	-33.403	12.236	1.00	14.73	A
ATOM	284	CG1	VAL	A	37	-12.146	-34.774	12.143	1.00	16.16	A
ATOM	285	CG2	VAL	A	37	-11.774	-32.274	12.445	1.00	14.31	A
ATOM	286	C	VAL	A	37	-14.508	-34.322	10.684	1.00	17.15	A
ATOM	287	O	VAL	A	37	-15.380	-34.665	11.495	1.00	16.68	A
ATOM	288	N	ALA	A	38	-14.325	-34.947	9.525	1.00	18.78	A
ATOM	289	CA	ALA	A	38	-15.146	-36.114	9.157	1.00	19.67	A
ATOM	290	CB	ALA	A	38	-16.354	-35.671	8.393	1.00	19.20	A
ATOM	291	C	ALA	A	38	-14.273	-36.995	8.288	1.00	21.68	A
ATOM	292	O	ALA	A	38	-13.526	-36.475	7.460	1.00	20.43	A
ATOM	293	N	ASP	A	39	-14.380	-38.312	8.476	1.00	23.51	A
ATOM	294	CA	ASP	A	39	-13.554	-39.266	7.746	1.00	27.39	A
ATOM	295	CB	ASP	A	39	-13.801	-39.139	6.244	1.00	30.92	A
ATOM	296	CG	ASP	A	39	-13.805	-40.490	5.533	1.00	35.17	A
ATOM	297	OD1	ASP	A	39	-13.575	-41.528	6.196	1.00	37.93	A
ATOM	298	OD2	ASP	A	39	-14.044	-40.515	4.303	1.00	38.02	A
ATOM	299	C	ASP	A	39	-12.136	-38.837	8.140	1.00	26.49	A
ATOM	300	O	ASP	A	39	-11.870	-38.606	9.310	1.00	29.24	A
ATOM	301	N	GLY	A	40	-11.226	-38.693	7.199	1.00	26.55	A
ATOM	302	CA	GLY	A	40	-9.893	-38.278	7.614	1.00	22.82	A
ATOM	303	C	GLY	A	40	-9.611	-36.884	7.084	1.00	20.99	A
ATOM	304	O	GLY	A	40	-8.488	-36.548	6.730	1.00	20.13	A
ATOM	305	N	THR	A	41	-10.640	-36.059	6.063	1.00	17.70	A
ATOM	306	CA	THR	A	41	-10.528	-34.735	6.493	1.00	17.27	A
ATOM	307	CB	THR	A	41	-11.407	-34.671	5.199	1.00	19.00	A
ATOM	308	OG1	THR	A	41	-11.050	-35.775	4.341	1.00	23.54	A
ATOM	309	CG2	THR	A	41	-11.215	-33.363	4.457	1.00	22.95	A
ATOM	310	C	THR	A	41	-10.974	-33.587	7.389	1.00	16.76	A
ATOM	311	O	THR	A	41	-11.921	-33.718	8.136	1.00	18.19	A
ATOM	312	N	LEU	A	42	-10.251	-32.483	7.333	1.00	14.51	A
ATOM	313	CA	LEU	A	42	-10.668	-31.272	8.035	1.00	13.60	A
ATOM	314	CB	LEU	A	42	-9.461	-30.576	8.698	1.00	14.21	A
ATOM	315	CG	LEU	A	42	-9.719	-29.130	9.112	1.00	12.61	A
ATOM	316	CD1	LEU	A	42	-10.808	-29.020	10.222	1.00	13.95	A
ATOM	317	CD2	LEU	A	42	-8.374	-28.566	9.579	1.00	15.96	A
ATOM	318	C	LEU	A	42	-11.170	-30.377	6.914	1.00	15.92	A
ATOM	319	O	LEU	A	42	-10.443	-30.104	5.951	1.00	15.29	A
ATOM	320	N	SER	A	43	-12.413	-29.907	7.016	1.00	13.67	A
ATOM	321	CA	SER	A	43	-12.914	-28.978	6.009	1.00	14.02	A
ATOM	322	CB	SER	A	43	-14.287	-29.408	5.461	1.00	15.11	A
ATOM	323	OG	SER	A	43	-14.202	-30.670	4.815	1.00	15.94	A
ATOM	324	C	SER	A	43	-13.020	-27.623	6.675	1.00	14.81	A
ATOM	325	O	SER	A	43	-13.360	-27.526	7.866	1.00	14.63	A
ATOM	326	N	LEU	A	44	-12.706	-26.571	5.928	1.00	13.45	A
ATOM	327	CA	LEU	A	44	-12.770	-25.220	6.475	1.00	13.96	A
ATOM	328	CB	LEU	A	44	-11.379	-24.576	6.501	1.00	16.23	A
ATOM	329	CG	LEU	A	44	-10.224	-25.221	7.264	1.00	19.59	A
ATOM	330	OD1	LEU	A	44	-10.661	-25.513	8.708	1.00	23.82	A
ATOM	331	OD2	LEU	A	44	-9.736	-26.446	6.550	1.00	22.21	A
ATOM	332	C	LEU	A	44	-13.643	-24.408	5.547	1.00	17.42	A
ATOM	333	O	LEU	A	44	-13.411	-24.421	4.336	1.00	17.59	A
ATOM	334	N	THR	A	45	-14.624	-23.682	6.087	1.00	15.58	A
ATOM	335	CA	THR	A	45	-15.517	-22.913	5.221	1.00	18.70	A
ATOM	336	CB	THR	A	45	-16.922	-23.570	5.153	1.00	18.52	A
ATOM	337	OG1	THR	A	45	-16.816	-24.941	4.706	1.00	18.50	A
ATOM	338	CG2	THR	A	45	-17.837	-22.792	4.165	1.00	18.61	A
ATOM	339	C	THR	A	45	-15.702	-21.465	5.653	1.00	19.93	A
ATOM	340	O	THR	A	45	-15.915	-21.185	6.844	1.00	20.27	A
ATOM	341	N	GLY	A	46	-15.617	-20.555	4.687	1.00	18.64	A
ATOM	342	CA	GLY	A	46	-15.837	-19.129	4.940	1.00	20.18	A
ATOM	343	CB	GLY	A	46	-17.022	-18.682	4.090	1.00	20.92	A
ATOM	344	C	GLY	A	46	-17.233	-19.247	3.011	1.00	20.00	A
ATOM	345	O	THR	A	47	-17.816	-17.692	4.537	1.00	20.46	A
ATOM	346	N	THR	A	47	-18.967	-17.267	3.729	1.00	22.40	A
ATOM	347	CB	THR	A	47	-20.188	-18.213	3.916	1.00	23.17	A
ATOM	348	OG1	THR	A	47	-21.242	-17.858	2.999	1.00	23.27	A
ATOM	349	CG2	THR	A	47	-20.745	-18.108	5.349	1.00	25.43	A
ATOM	350	C	THR	A	47	-19.440	-15.864	4.085	1.00	23.69	A
ATOM	351	O	THR	A	47	-19.201	-15.400	5.200	1.00	24.49	A
ATOM	352	N	ASP	A	48	-20.108	-15.199	3.149	1.00	23.27	A
ATOM	353	CA	ASP	A	48	-20.664	-13.857	3.407	1.00	22.37	A
ATOM	354	CB	ASP	A	48	-19.905	-12.780	2.621	1.00	24.34	A
ATOM	355	CG	ASP	A	48	-20.123	-12.864	1.121	1.00	24.11	A
ATOM	356	OD1	ASP	A	48	-20.826	-13.780	0.658	1.00	22.62	A
ATOM	357	OD2	ASP	A	48	-19.586	-12.001	0.407	1.00	28.57	A
ATOM	358	C	ASP	A	48	-22.155	-13.856	3.053	1.00	23.86	A
ATOM	359	O	ASP	A	48	-22.800	-12.787	2.957	1.00	22.46	A
ATOM	360	N	LEU	A	49	-22.690	-15.069	2.911	1.00	21.60	A
ATOM	361	CA	LEU	A	49	-24.084	-15.347	2.568	1.00	23.11	A
ATOM	362	CB	LEU	A	49	-25.043	-14.351	3.236	1.00	24.46	A
ATOM	363	CG	LEU	A	49	-25.225	-14.479	4.744	1.00	26.70	A
ATOM	364	CD1	LEU	A	49	-26.124	-13.337	5.190	1.00	27.13	A
ATOM	365	CD2	LEU	A	49	-25.795	-15.847	5.105	1.00	26.87	A

Figure 1 (continued 4)

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ATOM	366	C	LEU	A	49	-24.325	-15.305	1.067	1.00	20.63	A
ATOM	367	O	LEU	A	49	-25.268	-15.928	0.566	1.00	24.28	A
ATOM	368	N	GLU	A	50	-23.484	-14.575	0.346	1.00	19.18	A
ATOM	369	CA	GLU	A	50	-23.652	-14.494	-1.097	1.00	19.11	A
ATOM	370	CB	GLU	A	50	-23.243	-13.110	-1.610	1.00	21.43	A
ATOM	371	CG	GLU	A	50	-23.515	-12.896	-3.113	1.00	27.31	A
ATOM	372	CD	GLU	A	50	-23.235	-11.458	-3.604	1.00	28.85	A
ATOM	373	OE1	GLU	A	50	-22.085	-10.968	-3.454	1.00	31.33	A
ATOM	374	OE2	GLU	A	50	-24.168	-10.822	-4.172	1.00	31.83	A
ATOM	375	C	GLU	A	50	-22.787	-15.559	-1.758	1.00	20.12	A
ATOM	376	O	GLU	A	50	-23.166	-16.124	-2.786	1.00	19.05	A
ATOM	377	N	MET	A	51	-21.651	-15.846	-1.127	1.00	18.26	A
ATOM	378	CA	MET	A	51	-20.698	-16.832	-1.670	1.00	18.26	A
ATOM	379	CB	MET	A	51	-19.643	-16.116	-2.504	1.00	19.67	A
ATOM	380	CG	MET	A	51	-18.947	-15.032	-1.780	1.00	22.10	A
ATOM	381	SD	MET	A	51	-18.086	-14.041	-2.993	1.00	25.87	A
ATOM	382	CE	MET	A	51	-16.514	-14.275	-2.397	1.00	27.36	A
ATOM	383	C	MET	A	51	-20.053	-17.576	-0.525	1.00	18.84	A
ATOM	384	O	MET	A	51	-20.102	-17.129	0.634	1.00	18.64	A
ATOM	385	N	GLU	A	52	-19.428	-18.699	-0.853	1.00	16.68	A
ATOM	386	CA	GLU	A	52	-18.859	-19.572	0.152	1.00	19.13	A
ATOM	387	CB	GLU	A	52	-19.901	-20.637	0.452	1.00	22.65	A
ATOM	388	CG	GLU	A	52	-19.554	-21.806	1.323	1.00	32.13	A
ATOM	389	CD	GLU	A	52	-20.803	-22.623	1.650	1.00	34.31	A
ATOM	390	OE1	GLU	A	52	-20.682	-23.671	2.325	1.00	38.54	A
ATOM	391	OE2	GLU	A	52	-21.913	-22.211	1.235	1.00	36.05	A
ATOM	392	C	GLU	A	52	-17.595	-20.188	-0.449	1.00	18.25	A
ATOM	393	O	GLU	A	52	-17.555	-20.488	-1.639	1.00	17.91	A
ATOM	394	N	MET	A	53	-16.584	-20.356	0.377	1.00	18.60	A
ATOM	395	CA	MET	A	53	-15.339	-20.955	-0.074	1.00	17.33	A
ATOM	396	CB	MET	A	53	-14.202	-19.930	-0.036	1.00	21.43	A
ATOM	397	CG	MET	A	53	-12.851	-20.502	-0.484	1.00	26.15	A
ATOM	398	SD	MET	A	53	-12.771	-20.914	-2.256	1.00	32.73	A
ATOM	399	CE	MET	A	53	-12.410	-19.257	-2.959	1.00	30.62	A
ATOM	400	C	MET	A	53	-15.051	-22.112	0.886	1.00	17.68	A
ATOM	401	O	MET	A	53	-15.069	-21.933	2.102	1.00	17.40	A
ATOM	402	N	VAL	A	54	-14.786	-23.294	0.338	1.00	15.12	A
ATOM	403	CA	VAL	A	54	-14.507	-24.468	1.162	1.00	16.82	A
ATOM	404	CB	VAL	A	54	-15.508	-25.612	0.914	1.00	17.64	A
ATOM	405	CG1	VAL	A	54	-15.224	-26.754	1.871	1.00	18.47	A
ATOM	406	CG2	VAL	A	54	-16.959	-25.117	1.098	1.00	21.00	A
ATOM	407	C	VAL	A	54	-13.139	-25.036	0.823	1.00	17.33	A
ATOM	408	O	VAL	A	54	-12.814	-25.201	-0.343	1.00	19.27	A
ATOM	409	N	ALA	A	55	-12.349	-25.363	1.848	1.00	15.10	A
ATOM	410	CA	ALA	A	55	-11.031	-25.973	1.611	1.00	13.30	A
ATOM	411	CB	ALA	A	55	-9.923	-25.043	2.056	1.00	15.71	A
ATOM	412	C	ALA	A	55	-10.929	-27.286	2.394	1.00	16.85	A
ATOM	413	O	ALA	A	55	-11.528	-27.433	3.451	1.00	16.80	A
ATOM	414	N	ARG	A	56	-10.138	-28.233	1.895	1.00	15.48	A
ATOM	415	CA	ARG	A	56	-9.989	-29.505	2.613	1.00	15.80	A
ATOM	416	CB	ARG	A	56	-10.566	-30.677	1.789	1.00	20.20	A
ATOM	417	CG	ARG	A	56	-12.018	-30.440	1.349	1.00	23.44	A
ATOM	418	CD	ARG	A	56	-12.819	-31.720	1.096	1.00	28.95	A
ATOM	419	NE	ARG	A	56	-14.035	-31.591	1.909	1.00	31.67	A
ATOM	420	CE	ARG	A	56	-15.058	-30.787	1.625	1.00	32.95	A
ATOM	421	NH1	ARG	A	56	-15.053	-30.038	0.508	1.00	32.56	A
ATOM	422	NH2	ARG	A	56	-16.048	-30.668	2.503	1.00	29.00	A
ATOM	423	C	ARG	A	56	-8.515	-29.772	2.931	1.00	15.06	A
ATOM	424	O	ARG	A	56	-7.623	-29.430	2.131	1.00	16.17	A
ATOM	425	N	VAL	A	57	-8.273	-30.364	4.104	1.00	14.32	A
ATOM	426	CA	VAL	A	57	-6.919	-30.693	4.567	1.00	12.85	A
ATOM	427	CB	VAL	A	57	-6.481	-29.759	5.755	1.00	15.84	A
ATOM	428	CG1	VAL	A	57	-5.134	-30.198	6.297	1.00	17.83	A
ATOM	429	CG2	VAL	A	57	-6.452	-28.283	5.289	1.00	18.06	A
ATOM	430	C	VAL	A	57	-6.966	-32.141	5.049	1.00	13.46	A
ATOM	431	O	VAL	A	57	-7.853	-32.534	5.813	1.00	13.57	A
ATOM	432	N	ALA	A	58	-6.028	-32.968	4.596	1.00	12.91	A
ATOM	433	CA	ALA	A	58	-6.027	-34.351	5.050	1.00	13.63	A
ATOM	434	CB	ALA	A	58	-5.228	-35.213	4.062	1.00	16.31	A
ATOM	435	C	ALA	A	58	-5.423	-34.471	6.459	1.00	13.61	A
ATOM	436	O	ALA	A	58	-4.481	-33.740	6.807	1.00	15.06	A
ATOM	437	N	LEU	A	59	-5.997	-35.362	7.269	1.00	15.23	A
ATOM	438	CA	LEU	A	59	-5.558	-35.589	8.648	1.00	16.38	A
ATOM	439	CB	LEU	A	59	-6.748	-35.439	9.599	1.00	15.55	A
ATOM	440	CG	LEU	A	59	-7.384	-34.042	9.562	1.00	14.50	A
ATOM	441	CD1	LEU	A	59	-8.607	-34.021	10.509	1.00	15.98	A
ATOM	442	CD2	LEU	A	59	-6.364	-32.973	9.991	1.00	14.17	A
ATOM	443	C	LEU	A	59	-4.980	-36.986	8.804	1.00	20.00	A
ATOM	444	O	LEU	A	59	-5.702	-37.982	8.671	1.00	23.51	A
ATOM	445	N	VAL	A	60	-3.700	-37.070	9.138	1.00	20.91	A
ATOM	446	CA	VAL	A	60	-3.081	-38.379	9.305	1.00	22.99	A
ATOM	447	CB	VAL	A	60	-1.720	-38.472	8.532	1.00	21.30	A
ATOM	448	CG1	VAL	A	60	-0.726	-37.522	9.135	1.00	21.15	A
ATOM	449	CG2	VAL	A	60	-1.177	-39.910	8.545	1.00	24.79	A
ATOM	450	C	VAL	A	60	-2.861	-38.661	10.779	1.00	25.44	A
ATOM	451	O	VAL	A	60	-2.801	-39.830	11.197	1.00	26.02	A
ATOM	452	N	GLN	A	61	-2.761	-37.596	11.578	1.00	26.01	A
ATOM	453	CA	GLN	A	61	-2.551	-37.734	13.014	1.00	26.21	A
ATOM	454	CB	GLN	A	61	-1.962	-36.437	13.569	1.00	26.62	A
ATOM	455	CG	GLN	A	61	-0.643	-36.050	12.877	1.00	27.36	A
ATOM	456	CD	GLN	A	61	0.082	-34.866	13.534	1.00	29.51	A
ATOM	457	OE1	GLN	A	61	0.274	-34.851	14.750	1.00	30.47	A
ATOM	458	NE2	GLN	A	61	0.498	-33.881	12.726	1.00	28.34	A
ATOM	459	C	GLN	A	61	-3.893	-38.063	13.663	1.00	26.03	A
ATOM	460	O	GLN	A	61	-4.944	-37.822	13.065	1.00	26.37	A
ATOM	461	N	PRO	A	62	-3.878	-38.637	14.883	1.00	26.72	A
ATOM	462	CD	PRO	A	62	-2.749	-39.028	15.752	1.00	26.01	A
ATOM	463	CA	PRO	A	62	-5.159	-38.969	15.514	1.00	24.46	A
ATOM	464	CB	PRO	A	62	-4.758	-39.400	16.929	1.00	26.77	A
ATOM	465	CG	PRO	A	62	-3.406	-40.043	16.689	1.00	25.60	A

Figure 1 (continued 5)

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ATOM	466	C	PRO	A	62	-6.098	-37.789	15.500	1.00	21.59	A
ATOM	467	O	PRO	A	62	-5.693	-36.637	15.713	1.00	20.88	A
ATOM	468	N	HIS	A	63	-7.361	-38.082	15.234	1.00	21.18	A
ATOM	469	CA	HIS	A	63	-8.371	-37.046	15.179	1.00	17.84	A
ATOM	470	CB	HIS	A	63	-8.475	-36.482	13.754	1.00	18.27	A
ATOM	471	CG	HIS	A	63	-8.667	-37.536	12.708	1.00	18.43	A
ATOM	472	CD2	HIS	A	63	-9.792	-38.061	12.170	1.00	20.08	A
ATOM	473	ND1	HIS	A	63	-7.615	-38.203	12.120	1.00	20.69	A
ATOM	474	CE1	HIS	A	63	-8.083	-39.097	11.260	1.00	21.51	A
ATOM	475	NE2	HIS	A	63	-9.403	-39.030	11.272	1.00	22.48	A
ATOM	476	C	HIS	A	63	-9.728	-37.601	15.597	1.00	18.21	A
ATOM	477	O	HIS	A	63	-9.933	-38.834	15.643	1.00	20.01	A
ATOM	478	N	GLU	A	64	-10.643	-36.686	15.907	1.00	16.87	A
ATOM	479	CA	GLU	A	64	-11.993	-37.073	16.308	1.00	19.00	A
ATOM	480	CB	GLU	A	64	-12.160	-36.905	17.813	1.00	20.97	A
ATOM	481	CG	GLU	A	64	-11.224	-37.788	18.610	1.00	24.05	A
ATOM	482	CD	GLU	A	64	-11.335	-37.528	20.090	1.00	29.25	A
ATOM	483	OE1	GLU	A	64	-12.050	-36.577	20.463	1.00	30.33	A
ATOM	484	OE2	GLU	A	64	-10.710	-38.277	20.873	1.00	32.20	A
ATOM	485	C	GLU	A	64	-12.964	-36.181	15.567	1.00	17.16	A
ATOM	486	O	PRO	A	65	-12.753	-34.976	15.435	1.00	18.02	A
ATOM	487	N	PRO	A	65	-14.070	-36.758	15.084	1.00	17.24	A
ATOM	488	CA	PRO	A	65	-14.424	-38.180	15.166	1.00	17.26	A
ATOM	489	CB	PRO	A	65	-15.063	-35.988	14.344	1.00	16.23	A
ATOM	490	CG	PRO	A	65	-15.982	-37.053	13.753	1.00	16.65	A
ATOM	491	CD	PRO	A	65	-15.903	-38.171	14.775	1.00	17.89	A
ATOM	492	O	PRO	A	65	-15.825	-34.969	15.143	1.00	16.81	A
ATOM	493	N	GLY	A	66	-15.998	-35.076	16.372	1.00	18.43	A
ATOM	494	CA	GLY	A	66	-16.279	-33.965	14.415	1.00	16.40	A
ATOM	495	CB	GLY	A	66	-17.048	-32.905	15.003	1.00	16.58	A
ATOM	496	C	GLY	A	66	-16.925	-31.636	14.205	1.00	17.44	A
ATOM	497	O	ALA	A	66	-16.181	-31.543	13.219	1.00	18.08	A
ATOM	498	N	ALA	A	67	-17.655	-30.628	14.646	1.00	15.78	A
ATOM	499	CA	ALA	A	67	-17.660	-29.360	13.958	1.00	16.07	A
ATOM	500	CB	ALA	A	67	-18.734	-29.361	12.850	1.00	15.82	A
ATOM	501	C	ALA	A	67	-17.946	-28.232	14.919	1.00	17.46	A
ATOM	502	O	ALA	A	67	-18.623	-28.416	15.950	1.00	19.40	A
ATOM	503	N	THR	A	68	-17.433	-27.070	14.570	1.00	16.43	A
ATOM	504	CA	THR	A	68	-17.658	-25.853	15.337	1.00	16.34	A
ATOM	505	CB	THR	A	68	-16.788	-25.805	16.626	1.00	16.66	A
ATOM	506	OG1	THR	A	68	-17.221	-24.683	17.412	1.00	17.85	A
ATOM	507	CG2	THR	A	68	-15.312	-25.634	16.291	1.00	16.50	A
ATOM	508	C	THR	A	68	-17.290	-24.675	14.449	1.00	17.50	A
ATOM	509	O	THR	A	68	-16.857	-24.867	13.309	1.00	18.15	A
ATOM	510	N	THR	A	69	-17.492	-23.453	14.916	1.00	16.80	A
ATOM	511	CA	THR	A	69	-17.069	-22.299	14.121	1.00	16.22	A
ATOM	512	CB	THR	A	69	-18.267	-21.521	13.510	1.00	19.21	A
ATOM	513	OG1	THR	A	69	-18.868	-20.676	14.500	1.00	19.12	A
ATOM	514	CG2	THR	A	69	-19.314	-22.481	12.964	1.00	19.28	A
ATOM	515	C	THR	A	69	-16.254	-21.394	15.053	1.00	17.37	A
ATOM	516	O	THR	A	69	-16.542	-21.318	16.250	1.00	19.10	A
ATOM	517	N	VAL	A	70	-15.228	-20.743	14.523	1.00	16.92	A
ATOM	518	CA	VAL	A	70	-14.348	-19.854	15.311	1.00	16.96	A
ATOM	519	CB	VAL	A	70	-12.994	-20.555	15.682	1.00	18.01	A
ATOM	520	CG1	VAL	A	70	-13.223	-21.742	16.630	1.00	20.79	A
ATOM	521	CG2	VAL	A	70	-12.305	-21.010	14.414	1.00	18.76	A
ATOM	522	C	VAL	A	70	-14.000	-18.592	14.528	1.00	17.58	A
ATOM	523	O	PRO	A	71	-14.107	-18.570	13.284	1.00	16.41	A
ATOM	524	N	PRO	A	71	-13.576	-17.519	15.220	1.00	16.78	A
ATOM	525	CD	PRO	A	71	-13.582	-17.315	16.689	1.00	17.77	A
ATOM	526	CA	PRO	A	71	-13.224	-16.275	14.523	1.00	17.44	A
ATOM	527	CB	PRO	A	71	-12.701	-15.398	15.633	1.00	19.39	A
ATOM	528	CG	PRO	A	71	-13.616	-15.810	16.788	1.00	20.22	A
ATOM	529	C	PRO	A	71	-12.184	-16.546	13.451	1.00	17.20	A
ATOM	530	O	ALA	A	72	-11.091	-16.993	13.744	1.00	17.02	A
ATOM	531	N	ALA	A	72	-12.522	-16.251	12.204	1.00	16.42	A
ATOM	532	CA	ALA	A	72	-11.610	-16.566	11.126	1.00	16.85	A
ATOM	533	CB	ALA	A	72	-12.325	-16.376	9.776	1.00	18.54	A
ATOM	534	C	ALA	A	72	-10.294	-15.813	11.128	1.00	17.52	A
ATOM	535	O	ALA	A	72	-9.225	-16.433	10.975	1.00	17.07	A
ATOM	536	N	ARG	A	73	-10.342	-14.492	11.276	1.00	16.94	A
ATOM	537	CA	ARG	A	73	-9.109	-13.711	11.242	1.00	19.22	A
ATOM	538	CB	ARG	A	73	-9.394	-12.209	11.247	1.00	23.69	A
ATOM	539	CG	ARG	A	73	-8.138	-11.345	10.965	1.00	28.94	A
ATOM	540	CD	ARG	A	73	-7.648	-11.495	9.517	1.00	34.56	A
ATOM	541	NE	ARG	A	73	-6.218	-11.192	9.385	1.00	39.05	A
ATOM	542	CZ	ARG	A	73	-5.513	-11.337	8.262	1.00	40.82	A
ATOM	543	NH1	ARG	A	73	-6.102	-11.781	7.155	1.00	42.67	A
ATOM	544	NH2	ARG	A	73	-4.217	-11.044	8.246	1.00	41.48	A
ATOM	545	C	ARG	A	73	-8.202	-14.053	12.420	1.00	18.20	A
ATOM	546	O	ARG	A	73	-6.988	-14.203	12.260	1.00	17.86	A
ATOM	547	N	LYS	A	74	-8.794	-14.201	13.595	1.00	17.94	A
ATOM	548	CA	LYS	A	74	-7.998	-14.536	14.762	1.00	17.40	A
ATOM	549	CB	LYS	A	74	-8.853	-14.517	16.023	1.00	17.77	A
ATOM	550	CG	LYS	A	74	-9.201	-13.129	16.534	1.00	19.95	A
ATOM	551	CD	LYS	A	74	-10.300	-13.274	17.579	1.00	20.83	A
ATOM	552	CE	LYS	A	74	-10.701	-11.937	18.146	1.00	21.69	A
ATOM	553	NZ	LYS	A	74	-11.934	-12.085	18.959	1.00	18.53	A
ATOM	554	C	LYS	A	74	-7.364	-15.910	14.608	1.00	15.84	A
ATOM	555	O	LYS	A	74	-6.181	-16.077	14.902	1.00	16.97	A
ATOM	556	N	PHE	A	75	-8.128	-16.896	14.144	1.00	16.01	A
ATOM	557	CA	PHE	A	75	-7.565	-18.241	13.996	1.00	16.50	A
ATOM	558	CB	PHE	A	75	-8.667	-19.271	13.657	1.00	15.00	A
ATOM	559	CG	PHE	A	75	-8.176	-20.690	13.548	1.00	17.05	A
ATOM	560	CD1	PHE	A	75	-7.463	-21.292	14.585	1.00	18.49	A
ATOM	561	CD2	PHE	A	75	-8.449	-21.441	12.409	1.00	18.78	A
ATOM	562	CE1	PHE	A	75	-7.031	-22.619	14.485	1.00	19.50	A
ATOM	563	CE2	PHE	A	75	-8.011	-22.784	12.300	1.00	20.42	A
ATOM	564	CZ	PHE	A	75	-7.303	-23.364	13.339	1.00	17.99	A
ATOM	565	C	PHE	A	75	-6.451	-18.217	12.947	1.00	15.71	A

Figure 1 (continued 6)

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ATOM	566	O	PHE	A	75	-5.377	-18.772	13.158	1.00	15.69	A
ATOM	567	N	PHE	A	76	-6.671	-17.524	11.821	1.00	15.86	A
ATOM	568	CA	PHE	A	76	-5.625	-17.426	10.800	1.00	15.67	A
ATOM	569	CB	PHE	A	76	-6.182	-16.680	9.572	1.00	16.48	A
ATOM	570	CG	PHE	A	76	-5.186	-16.476	8.472	1.00	20.93	A
ATOM	571	CD1	PHE	A	76	-4.368	-17.506	8.049	1.00	20.82	A
ATOM	572	CD2	PHE	A	76	-5.108	-15.250	7.830	1.00	25.97	A
ATOM	573	CE1	PHE	A	76	-3.481	-17.330	6.996	1.00	22.93	A
ATOM	574	CE2	PHE	A	76	-4.219	-15.058	6.761	1.00	27.38	A
ATOM	575	CZ	PHE	A	76	-3.407	-16.104	6.348	1.00	24.82	A
ATOM	576	CO	PHE	A	76	-4.366	-16.709	11.335	1.00	16.51	A
ATOM	577	ON	PHE	A	76	-3.244	-17.182	11.129	1.00	15.99	A
ATOM	578	N	ASP	A	77	-4.544	-15.583	12.027	1.00	14.50	A
ATOM	579	CA	ASP	A	77	-3.387	-14.859	12.560	1.00	17.13	A
ATOM	580	CB	ASP	A	77	-3.832	-13.526	13.167	1.00	19.74	A
ATOM	581	CG	ASP	A	77	-4.227	-12.510	12.107	1.00	23.30	A
ATOM	582	OD1	ASP	A	77	-3.860	-12.698	10.926	1.00	23.00	A
ATOM	583	OD2	ASP	A	77	-4.897	-11.515	12.465	1.00	24.82	A
ATOM	584	O	ASP	A	77	-2.618	-15.695	13.590	1.00	16.29	A
ATOM	585	C	ASP	A	77	-1.399	-15.629	13.647	1.00	16.00	A
ATOM	586	N	ILE	A	78	-3.325	-16.465	14.414	1.00	15.43	A
ATOM	587	CA	ILE	A	78	-2.633	-17.306	15.393	1.00	15.62	A
ATOM	588	CB	ILE	A	78	-3.649	-18.030	16.297	1.00	16.32	A
ATOM	589	CG2	ILE	A	78	-2.968	-19.174	17.072	1.00	17.56	A
ATOM	590	CG1	ILE	A	78	-4.258	-17.015	17.275	1.00	17.00	A
ATOM	591	CD1	ILE	A	78	-5.491	-17.573	18.024	1.00	17.64	A
ATOM	592	C	ILE	A	78	-1.809	-18.354	14.652	1.00	16.31	A
ATOM	593	O	ILE	A	78	-0.634	-18.563	14.949	1.00	16.75	A
ATOM	594	N	CYS	A	79	-2.413	-19.013	13.676	1.00	14.73	A
ATOM	595	CA	CYS	A	79	-1.655	-20.046	12.938	1.00	15.03	A
ATOM	596	CB	CYS	A	79	-2.603	-20.761	11.979	1.00	16.89	A
ATOM	597	SC	CYS	A	79	-3.823	-21.817	12.844	1.00	17.54	A
ATOM	598	C	CYS	A	79	-0.456	-19.455	12.192	1.00	16.05	A
ATOM	599	O	CYS	A	79	0.649	-19.988	12.265	1.00	17.02	A
ATOM	600	N	ARG	A	80	-0.669	-18.337	11.512	1.00	16.19	A
ATOM	601	CA	ARG	A	80	0.393	-17.690	10.775	1.00	16.85	A
ATOM	602	CB	ARG	A	80	-0.188	-16.537	9.946	1.00	20.00	A
ATOM	603	CG	ARG	A	80	0.778	-15.991	8.885	1.00	27.92	A
ATOM	604	CD	ARG	A	80	0.031	-15.082	7.905	1.00	32.53	A
ATOM	605	NE	ARG	A	80	-0.726	-14.049	8.612	1.00	35.79	A
ATOM	606	CZ	ARG	A	80	-0.172	-13.067	9.323	1.00	37.31	A
ATOM	607	NH1	ARG	A	80	1.152	-12.973	9.420	1.00	38.32	A
ATOM	608	NH2	ARG	A	80	-0.944	-12.190	9.956	1.00	37.64	A
ATOM	609	C	ARG	A	80	1.494	-17.166	11.704	1.00	15.48	A
ATOM	610	O	ARG	A	80	2.671	-17.183	11.330	1.00	16.18	A
ATOM	611	N	GLY	A	81	1.126	-16.734	12.920	1.00	13.81	A
ATOM	612	CA	GLY	A	81	2.092	-16.185	13.853	1.00	15.77	A
ATOM	613	C	GLY	A	81	2.971	-17.205	14.540	1.00	15.13	A
ATOM	614	O	GLY	A	81	3.993	-16.858	15.138	1.00	15.06	A
ATOM	615	N	LEU	A	82	2.558	-18.463	14.470	1.00	13.35	A
ATOM	616	CA	LEU	A	82	3.351	-19.550	15.059	1.00	13.35	A
ATOM	617	CB	LEU	A	82	2.525	-20.845	15.156	1.00	12.49	A
ATOM	618	CG	LEU	A	82	1.493	-20.791	16.304	1.00	12.47	A
ATOM	619	CD1	LEU	A	82	0.486	-21.910	16.176	1.00	12.91	A
ATOM	620	CD2	LEU	A	82	2.215	-20.852	17.693	1.00	14.10	A
ATOM	621	C	LEU	A	82	4.565	-19.749	14.158	1.00	15.03	A
ATOM	622	O	LEU	A	82	4.527	-19.404	12.963	1.00	15.46	A
ATOM	623	N	PRO	A	83	5.645	-20.316	14.709	1.00	16.44	A
ATOM	624	CA	PRO	A	83	5.747	-20.916	16.057	1.00	16.82	A
ATOM	625	CB	PRO	A	83	6.868	-20.532	13.940	1.00	17.96	A
ATOM	626	CG	PRO	A	83	7.878	-20.913	15.013	1.00	17.93	A
ATOM	627	C	PRO	A	83	7.049	-21.726	15.978	1.00	17.83	A
ATOM	628	O	PRO	A	83	6.792	-21.560	12.827	1.00	19.15	A
ATOM	629	N	GLU	A	84	5.974	-22.483	12.842	1.00	16.64	A
ATOM	630	CA	GLU	A	84	7.647	-21.362	11.834	1.00	18.77	A
ATOM	631	CB	GLU	A	84	7.720	-22.297	10.724	1.00	20.63	A
ATOM	632	CG	GLU	A	84	8.866	-21.879	9.798	1.00	23.64	A
ATOM	633	CD	GLU	A	84	9.092	-22.783	8.594	1.00	31.62	A
ATOM	634	OE1	GLU	A	84	10.336	-22.356	7.829	1.00	36.15	A
ATOM	635	OE2	GLU	A	84	10.445	-21.139	7.504	1.00	39.83	A
ATOM	636	C	GLU	A	84	11.206	-23.221	7.567	1.00	40.03	A
ATOM	637	O	GLU	A	84	7.978	-23.693	11.297	1.00	19.73	A
ATOM	638	N	GLU	A	84	8.801	-23.867	12.213	1.00	20.17	A
ATOM	639	CA	GLY	A	85	7.262	-24.686	10.779	1.00	20.11	A
ATOM	640	C	GLY	A	85	7.432	-26.046	11.263	1.00	19.52	A
ATOM	641	O	GLY	A	85	6.582	-26.430	12.465	1.00	19.27	A
ATOM	642	N	ALA	A	86	6.600	-27.576	12.919	1.00	21.77	A
ATOM	643	CA	ALA	A	86	5.825	-25.479	12.996	1.00	16.80	A
ATOM	644	CB	ALA	A	86	4.989	-25.776	14.152	1.00	16.45	A
ATOM	645	C	ALA	A	86	4.313	-24.490	14.661	1.00	16.16	A
ATOM	646	O	ALA	A	86	3.910	-26.805	13.839	1.00	16.34	A
ATOM	647	N	GLU	A	87	3.430	-26.884	12.703	1.00	16.48	A
ATOM	648	CA	GLU	A	87	3.552	-27.584	14.857	1.00	15.82	A
ATOM	649	CB	GLU	A	87	2.479	-28.577	14.792	1.00	16.94	A
ATOM	650	CG	GLU	A	87	2.871	-29.867	15.511	1.00	20.12	A
ATOM	651	CD	GLU	A	87	3.869	-30.727	14.757	1.00	24.42	A
ATOM	652	OE1	GLU	A	87	3.204	-31.527	13.643	1.00	29.00	A
ATOM	653	OE2	GLU	A	87	1.962	-31.445	13.512	1.00	30.19	A
ATOM	654	C	GLU	A	87	3.927	-32.242	12.902	1.00	33.75	A
ATOM	655	O	GLU	A	87	1.371	-27.889	15.598	1.00	16.68	A
ATOM	656	N	ILE	A	88	1.643	-27.315	16.669	1.00	16.47	A
ATOM	657	CA	ILE	A	88	0.137	-27.956	15.112	1.00	15.63	A
ATOM	658	CB	ILE	A	88	-0.964	-27.286	15.783	1.00	14.47	A
ATOM	659	CG2	ILE	A	88	-1.551	-26.225	14.815	1.00	14.61	A
ATOM	660	CG1	ILE	A	88	-2.717	-25.471	15.455	1.00	15.66	A
ATOM	661	CD1	ILE	A	88	-0.434	-25.252	14.413	1.00	16.03	A
ATOM	662	O	ILE	A	88	-0.916	-24.176	13.495	1.00	15.45	A
ATOM	663	N	ALA	A	89	-2.026	-28.285	16.215	1.00	13.85	A
ATOM	664	CA	ALA	A	89	-2.626	-28.982	15.376	1.00	14.57	A
ATOM	665	CB	ALA	A	89	-2.251	-28.360	17.529	1.00	12.25	A

Figure 1 (continued 7)

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ATOM	666	CA	ALA	A	89	-3.239	-29.289	18.093	1.00	12.02	A
ATOM	667	CB	ALA	A	89	-2.659	-29.952	19.353	1.00	13.11	A
ATOM	668	C	ALA	A	89	-4.472	-28.479	18.426	1.00	11.71	A
ATOM	669	O	ALA	A	89	-4.399	-27.426	19.061	1.00	13.67	A
ATOM	670	N	VAL	A	90	-5.626	-28.961	18.000	1.00	10.89	A
ATOM	671	CA	VAL	A	90	-6.867	-28.214	18.186	1.00	12.44	A
ATOM	672	CB	VAL	A	90	-7.383	-27.710	16.811	1.00	12.40	A
ATOM	673	CG1	VAL	A	90	-8.769	-27.064	16.940	1.00	13.53	A
ATOM	674	CG2	VAL	A	90	-6.412	-26.706	16.235	1.00	14.45	A
ATOM	675	C	VAL	A	90	-7.922	-29.131	18.759	1.00	13.45	A
ATOM	676	O	VAL	A	90	-8.095	-30.261	18.298	1.00	15.19	A
ATOM	677	N	GLN	A	91	-8.636	-28.655	19.774	1.00	14.36	A
ATOM	678	CA	GLN	A	91	-9.735	-29.465	20.314	1.00	14.06	A
ATOM	679	CB	GLN	A	91	-9.285	-30.386	21.450	1.00	17.88	A
ATOM	680	CG	GLN	A	91	-8.554	-29.714	22.519	1.00	21.85	A
ATOM	681	CD	GLN	A	91	-7.719	-30.667	23.362	1.00	28.08	A
ATOM	682	OE1	GLN	A	91	-7.236	-31.706	22.883	1.00	32.53	A
ATOM	683	NE2	GLN	A	91	-7.514	-30.297	24.610	1.00	28.96	A
ATOM	684	C	GLN	A	91	-10.861	-28.572	20.778	1.00	15.88	A
ATOM	685	O	GLN	A	91	-10.662	-27.498	21.336	1.00	15.55	A
ATOM	686	N	LEU	A	92	-12.076	-29.022	20.506	1.00	15.92	A
ATOM	687	CA	LEU	A	92	-13.242	-28.290	20.937	1.00	18.46	A
ATOM	688	CB	LEU	A	92	-14.426	-28.669	20.044	1.00	18.53	A
ATOM	689	CG	LEU	A	92	-15.797	-28.084	20.379	1.00	19.11	A
ATOM	690	CD1	LEU	A	92	-15.815	-26.567	20.190	1.00	17.67	A
ATOM	691	CD2	LEU	A	92	-16.801	-28.748	19.451	1.00	19.82	A
ATOM	692	C	LEU	A	92	-13.490	-28.723	22.370	1.00	19.94	A
ATOM	693	O	LEU	A	92	-13.491	-29.938	22.675	1.00	20.27	A
ATOM	694	N	GLU	A	93	-13.692	-27.737	23.242	1.00	21.27	A
ATOM	695	CA	GLU	A	93	-13.950	-27.969	24.656	1.00	23.60	A
ATOM	696	CB	GLU	A	93	-12.727	-27.593	25.472	1.00	24.28	A
ATOM	697	CG	GLU	A	93	-11.502	-28.346	25.001	1.00	25.20	A
ATOM	698	CD	GLU	A	93	-10.402	-28.368	26.037	1.00	26.28	A
ATOM	699	OE1	GLU	A	93	-10.239	-27.343	26.732	1.00	28.86	A
ATOM	700	OE2	GLU	A	93	-9.701	-29.405	26.152	1.00	26.10	A
ATOM	701	C	GLU	A	93	-15.122	-27.105	25.061	1.00	24.07	A
ATOM	702	O	GLU	A	93	-14.943	-26.031	25.640	1.00	25.47	A
ATOM	703	N	GLY	A	94	-16.318	-27.570	24.726	1.00	26.68	A
ATOM	704	CA	GLY	A	94	-17.517	-26.822	25.063	1.00	28.20	A
ATOM	705	C	GLY	A	94	-17.675	-25.520	24.310	1.00	28.08	A
ATOM	706	O	GLY	A	94	-17.807	-25.500	23.080	1.00	30.95	A
ATOM	707	N	GLU	A	95	-17.668	-24.409	25.036	1.00	27.27	A
ATOM	708	CA	GLU	A	95	-17.840	-23.109	24.405	1.00	26.17	A
ATOM	709	CB	GLU	A	95	-18.429	-22.111	25.404	1.00	29.49	A
ATOM	710	CG	GLU	A	95	-19.812	-22.514	25.947	1.00	34.68	A
ATOM	711	CD	GLU	A	95	-20.819	-22.776	24.829	1.00	37.59	A
ATOM	712	OE1	GLU	A	95	-20.860	-21.971	23.871	1.00	39.61	A
ATOM	713	OE2	GLU	A	95	-21.568	-23.779	24.915	1.00	40.32	A
ATOM	714	C	GLU	A	95	-16.561	-22.524	23.816	1.00	23.92	A
ATOM	715	O	GLU	A	95	-16.603	-21.458	23.201	1.00	24.33	A
ATOM	716	N	ARG	A	96	-15.429	-23.192	24.031	1.00	19.97	A
ATOM	717	CA	ARG	A	96	-14.189	-22.685	23.489	1.00	18.11	A
ATOM	718	CB	ARG	A	96	-13.242	-22.189	24.619	1.00	20.61	A
ATOM	719	CG	ARG	A	96	-12.680	-23.267	25.616	1.00	22.85	A
ATOM	720	CD	ARG	A	96	-11.343	-23.897	25.139	1.00	25.49	A
ATOM	721	NE	ARG	A	96	-10.623	-24.711	26.143	1.00	24.91	A
ATOM	722	CZ	ARG	A	96	-9.771	-24.241	27.058	1.00	25.23	A
ATOM	723	NH1	ARG	A	96	-9.515	-22.942	27.120	1.00	26.05	A
ATOM	724	NH2	ARG	A	96	-9.147	-25.086	27.903	1.00	20.77	A
ATOM	725	C	ARG	A	96	-13.471	-23.726	22.666	1.00	15.35	A
ATOM	726	O	ARG	A	96	-13.740	-24.924	22.790	1.00	15.87	A
ATOM	727	N	MET	A	97	-12.609	-23.237	21.781	1.00	14.95	A
ATOM	728	CA	MET	A	97	-11.789	-24.134	20.978	1.00	12.81	A
ATOM	729	CB	MET	A	97	-11.921	-23.850	19.476	1.00	15.67	A
ATOM	730	CG	MET	A	97	-11.205	-24.939	18.666	1.00	13.94	A
ATOM	731	SD	MET	A	97	-11.365	-24.789	16.864	1.00	16.92	A
ATOM	732	CE	MET	A	97	-9.931	-23.715	16.512	1.00	14.97	A
ATOM	733	C	MET	A	97	-10.377	-23.860	21.444	1.00	12.28	A
ATOM	734	O	MET	A	97	-9.912	-22.714	21.373	1.00	13.91	A
ATOM	735	N	LEU	A	98	-9.697	-24.908	21.922	1.00	11.68	A
ATOM	736	CA	LEU	A	98	-8.342	-24.751	22.424	1.00	11.70	A
ATOM	737	CB	LEU	A	98	-8.137	-25.671	23.643	1.00	13.52	A
ATOM	738	CG	LEU	A	98	-6.728	-25.651	24.249	1.00	15.75	A
ATOM	739	CD1	LEU	A	98	-6.406	-24.288	24.856	1.00	16.82	A
ATOM	740	CD2	LEU	A	98	-6.635	-26.764	25.314	1.00	17.18	A
ATOM	741	C	LEU	A	98	-7.340	-25.091	21.327	1.00	11.06	A
ATOM	742	O	LEU	A	98	-7.413	-26.162	20.715	1.00	13.52	A
ATOM	743	N	VAL	A	99	-6.429	-24.155	21.081	1.00	11.82	A
ATOM	744	CA	VAL	A	99	-5.357	-24.306	20.102	1.00	10.73	A
ATOM	745	CB	VAL	A	99	-5.348	-23.106	19.112	1.00	10.91	A
ATOM	746	CG1	VAL	A	99	-4.236	-23.307	18.079	1.00	13.86	A
ATOM	747	CG2	VAL	A	99	-6.690	-23.022	18.393	1.00	13.77	A
ATOM	748	C	VAL	A	99	-4.032	-24.330	20.855	1.00	11.36	A
ATOM	749	O	VAL	A	99	-3.735	-23.418	21.637	1.00	12.82	A
ATOM	750	N	ARG	A	100	-3.241	-25.378	20.621	1.00	11.29	A
ATOM	751	CA	ARG	A	100	-1.951	-25.515	21.299	1.00	10.63	A
ATOM	752	CB	ARG	A	100	-2.017	-26.687	22.287	1.00	12.67	A
ATOM	753	CG	ARG	A	100	-3.028	-26.536	23.444	1.00	13.82	A
ATOM	754	CD	ARG	A	100	-2.999	-27.792	24.309	1.00	18.46	A
ATOM	755	NE	ARG	A	100	-3.557	-28.927	23.578	1.00	18.43	A
ATOM	756	CZ	ARG	A	100	-2.969	-30.114	23.447	1.00	20.90	A
ATOM	757	NH1	ARG	A	100	-1.779	-30.341	24.003	1.00	23.86	A
ATOM	758	NH2	ARG	A	100	-3.571	-31.076	22.763	1.00	21.35	A
ATOM	759	C	ARG	A	100	-0.818	-25.796	20.348	1.00	12.06	A
ATOM	760	O	ARG	A	100	-0.952	-26.607	19.455	1.00	13.88	A
ATOM	761	N	SER	A	101	0.319	-25.142	20.560	1.00	10.58	A
ATOM	762	CA	SER	A	101	1.500	-25.414	19.734	1.00	12.72	A
ATOM	763	CB	SER	A	101	1.457	-24.582	18.448	1.00	14.43	A
ATOM	764	OG	SER	A	101	2.562	-24.907	17.600	1.00	14.52	A
ATOM	765	C	SER	A	101	2.697	-25.036	20.597	1.00	13.21	A

Figure 1 (continued 8)

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ATOM	766	O	SER	A	101	2.755	-23.917	21.070	1.00	12.38	A
ATOM	767	N	GLY	A	102	3.655	-25.952	20.787	1.00	14.97	A
ATOM	768	CA	GLY	A	102	4.787	-25.626	21.655	1.00	15.35	A
ATOM	769	C	GLY	A	102	4.234	-25.239	23.022	1.00	14.72	A
ATOM	770	O	GLY	A	102	3.396	-25.957	23.566	1.00	15.06	A
ATOM	771	N	ARG	A	103	4.715	-24.127	23.580	1.00	14.39	A
ATOM	772	CA	ARG	A	103	4.225	-23.632	24.861	1.00	15.53	A
ATOM	773	CB	ARG	A	103	5.383	-23.301	25.800	1.00	16.98	A
ATOM	774	CG	ARG	A	103	6.122	-24.596	26.170	1.00	18.28	A
ATOM	775	CD	ARG	A	103	7.074	-24.407	27.335	1.00	22.26	A
ATOM	776	NE	ARG	A	103	8.146	-23.480	27.027	1.00	24.02	A
ATOM	777	CZ	ARG	A	103	9.048	-23.096	27.930	1.00	27.13	A
ATOM	778	NH1	ARG	A	103	8.986	-23.567	29.177	1.00	28.33	A
ATOM	779	NH2	ARG	A	103	10.000	-22.243	27.594	1.00	29.41	A
ATOM	780	C	ARG	A	103	3.346	-22.402	24.617	1.00	15.01	A
ATOM	781	O	ARG	A	103	3.318	-21.450	25.423	1.00	16.19	A
ATOM	782	N	SER	A	104	2.650	-22.424	23.477	1.00	12.66	A
ATOM	783	CA	SER	A	104	1.707	-21.349	23.143	1.00	11.12	A
ATOM	784	CB	SER	A	104	1.917	-20.857	21.705	1.00	11.60	A
ATOM	785	OG	SER	A	104	3.262	-20.458	21.462	1.00	11.97	A
ATOM	786	C	SER	A	104	0.313	-21.971	23.254	1.00	13.02	A
ATOM	787	O	SER	A	104	0.076	-23.082	22.774	1.00	13.52	A
ATOM	788	N	ARG	A	105	-0.608	-21.251	23.895	1.00	11.22	A
ATOM	789	CA	ARG	A	105	-1.991	-21.722	24.070	1.00	13.13	A
ATOM	790	CB	ARG	A	105	-2.262	-22.132	25.534	1.00	14.88	A
ATOM	791	CG	ARG	A	105	-1.481	-23.313	26.011	1.00	14.45	A
ATOM	792	CD	ARG	A	105	-1.618	-23.515	27.546	1.00	14.09	A
ATOM	793	NE	ARG	A	105	-3.010	-23.510	28.001	1.00	16.53	A
ATOM	794	CZ	ARG	A	105	-3.784	-24.593	28.018	1.00	18.83	A
ATOM	795	NH1	ARG	A	105	-3.293	-25.743	27.603	1.00	17.38	A
ATOM	796	NH2	ARG	A	105	-5.054	-24.513	28.441	1.00	18.17	A
ATOM	797	C	ARG	A	105	-2.956	-20.617	23.727	1.00	13.13	A
ATOM	798	O	ARG	A	105	-2.750	-19.454	24.098	1.00	13.47	A
ATOM	799	N	PHE	A	106	-4.036	-20.973	23.032	1.00	11.95	A
ATOM	800	CA	PHE	A	106	-5.055	-19.984	22.687	1.00	12.74	A
ATOM	801	CB	PHE	A	106	-4.909	-19.554	21.211	1.00	12.74	A
ATOM	802	CG	PHE	A	106	-3.507	-19.127	20.851	1.00	13.12	A
ATOM	803	CD1	PHE	A	106	-2.537	-20.086	20.549	1.00	13.32	A
ATOM	804	CD2	PHE	A	106	-3.146	-17.791	20.918	1.00	13.88	A
ATOM	805	CE1	PHE	A	106	-1.230	-19.724	20.331	1.00	13.59	A
ATOM	806	CE2	PHE	A	106	-1.819	-17.406	20.702	1.00	15.45	A
ATOM	807	CZ	PHE	A	106	-0.862	-18.385	20.411	1.00	13.62	A
ATOM	808	C	PHE	A	106	-6.422	-20.606	22.881	1.00	12.43	A
ATOM	809	O	PHE	A	106	-6.666	-21.731	22.464	1.00	13.63	A
ATOM	810	N	SER	A	107	-7.322	-19.864	23.519	1.00	12.50	A
ATOM	811	CA	SER	A	107	-8.683	-20.348	23.707	1.00	15.61	A
ATOM	812	CB	SER	A	107	-9.056	-20.308	25.183	1.00	17.07	A
ATOM	813	OG	SER	A	107	-10.401	-20.709	25.398	1.00	20.88	A
ATOM	814	C	SER	A	107	-9.551	-19.357	22.940	1.00	14.70	A
ATOM	815	O	SER	A	107	-9.596	-18.184	23.304	1.00	15.97	A
ATOM	816	N	LEU	A	108	-10.219	-19.841	21.882	1.00	15.80	A
ATOM	817	CA	LEU	A	108	-11.072	-19.012	21.039	1.00	15.44	A
ATOM	818	CB	LEU	A	108	-10.829	-19.356	19.565	1.00	14.95	A
ATOM	819	CG	LEU	A	108	-9.457	-18.953	19.034	1.00	15.14	A
ATOM	820	CD1	LEU	A	108	-9.221	-19.543	17.631	1.00	17.32	A
ATOM	821	CD2	LEU	A	108	-9.368	-17.437	19.028	1.00	18.64	A
ATOM	822	C	LEU	A	108	-12.548	-19.248	21.305	1.00	14.24	A
ATOM	823	O	LEU	A	108	-12.949	-20.357	21.612	1.00	14.91	A
ATOM	824	N	SER	A	109	-13.347	-18.194	21.121	1.00	16.51	A
ATOM	825	CA	SER	A	109	-14.789	-18.290	21.304	1.00	16.82	A
ATOM	826	CB	SER	A	109	-15.426	-16.899	21.319	1.00	19.43	A
ATOM	827	OG	SER	A	109	-15.108	-16.215	20.106	1.00	24.23	A
ATOM	828	C	SER	A	109	-15.367	-19.064	20.138	1.00	17.73	A
ATOM	829	O	SER	A	109	-14.799	-19.072	19.056	1.00	18.59	A
ATOM	830	N	THR	A	110	-16.485	-19.728	20.364	1.00	16.33	A
ATOM	831	CA	THR	A	110	-17.113	-20.485	19.277	1.00	17.92	A
ATOM	832	CB	THR	A	110	-17.101	-22.013	19.518	1.00	18.59	A
ATOM	833	OG1	THR	A	110	-17.879	-22.330	20.685	1.00	19.81	A
ATOM	834	CG2	THR	A	110	-15.654	-22.546	19.697	1.00	17.30	A
ATOM	835	C	THR	A	110	-18.572	-20.118	19.136	1.00	19.22	A
ATOM	836	O	THR	A	110	-19.167	-19.492	20.023	1.00	17.85	A
ATOM	837	N	LEU	A	111	-19.124	-20.499	17.991	1.00	18.88	A
ATOM	838	CA	LEU	A	111	-20.553	-20.351	17.716	1.00	19.64	A
ATOM	839	CB	LEU	A	111	-20.847	-19.228	16.737	1.00	19.79	A
ATOM	840	CG	LEU	A	111	-20.773	-17.810	17.316	1.00	19.24	A
ATOM	841	CD1	LEU	A	111	-20.926	-16.832	16.218	1.00	19.44	A
ATOM	842	CD2	LEU	A	111	-21.882	-17.599	18.408	1.00	20.76	A
ATOM	843	C	LEU	A	111	-20.887	-21.715	17.112	1.00	20.43	A
ATOM	844	O	LEU	A	111	-20.073	-22.344	16.402	1.00	18.31	A
ATOM	845	N	PRO	A	112	-22.085	-22.222	17.394	1.00	19.50	A
ATOM	846	CD	PRO	A	112	-23.083	-21.651	18.318	1.00	20.92	A
ATOM	847	CA	PRO	A	112	-22.523	-23.525	16.899	1.00	20.93	A
ATOM	848	CB	PRO	A	112	-23.959	-23.605	17.391	1.00	22.46	A
ATOM	849	CG	PRO	A	112	-23.884	-22.845	18.660	1.00	21.60	A
ATOM	850	C	PRO	A	112	-22.421	-23.751	15.398	1.00	20.94	A
ATOM	851	O	PRO	A	112	-22.767	-22.888	14.582	1.00	21.16	A
ATOM	852	N	ALA	A	113	-21.904	-24.922	15.040	1.00	22.00	A
ATOM	853	CA	ALA	A	113	-21.786	-25.266	13.625	1.00	23.34	A
ATOM	854	CB	ALA	A	113	-21.161	-26.665	13.485	1.00	22.78	A
ATOM	855	C	ALA	A	113	-23.191	-25.235	13.006	1.00	25.52	A
ATOM	856	O	ALA	A	113	-23.369	-24.901	11.826	1.00	24.33	A
ATOM	857	N	ALA	A	114	-24.191	-25.575	13.812	1.00	26.80	A
ATOM	858	CA	ALA	A	114	-25.576	-25.561	13.345	1.00	29.81	A
ATOM	859	CB	ALA	A	114	-26.479	-26.091	14.435	1.00	29.86	A
ATOM	860	C	ALA	A	114	-26.049	-24.167	12.904	1.00	31.08	A
ATOM	861	O	ALA	A	114	-27.019	-24.040	12.146	1.00	32.98	A
ATOM	862	N	ASP	A	115	-25.366	-23.127	13.370	1.00	31.48	A
ATOM	863	CA	ASP	A	115	-25.706	-21.738	13.046	1.00	30.69	A
ATOM	864	CB	ASP	A	115	-25.221	-20.795	14.150	1.00	32.52	A
ATOM	865	CG	ASP	A	115	-25.969	-20.954	15.464	1.00	33.04	A

Figure 1 (continued 9)

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ATOM	866	OD1	ASP	A	115	-26.756	-21.906	15.653	1.00	34.66	A
ATOM	867	OD2	ASP	A	115	-25.737	-20.092	16.336	1.00	36.15	A
ATOM	868	C	ASP	A	115	-25.058	-21.240	11.764	1.00	31.41	A
ATOM	869	O	ASP	A	115	-25.450	-20.196	11.235	1.00	30.02	A
ATOM	870	N	PHE	A	116	-24.038	-21.951	11.286	1.00	30.62	A
ATOM	871	CA	PHE	A	116	-23.315	-21.513	10.102	1.00	31.36	A
ATOM	872	CB	PHE	A	116	-22.046	-22.362	9.881	1.00	29.27	A
ATOM	873	CG	PHE	A	116	-20.991	-21.658	9.069	1.00	27.56	A
ATOM	874	CD1	PHE	A	116	-20.203	-20.670	9.641	1.00	27.11	A
ATOM	875	CD2	PHE	A	116	-20.805	-21.958	7.721	1.00	27.96	A
ATOM	876	CE1	PHE	A	116	-19.246	-19.982	8.889	1.00	28.16	A
ATOM	877	CE2	PHE	A	116	-19.855	-21.280	6.963	1.00	28.67	A
ATOM	878	CZ	PHE	A	116	-19.071	-20.288	7.546	1.00	29.11	A
ATOM	879	C	PHE	A	116	-24.191	-21.561	8.863	1.00	33.68	A
ATOM	880	O	PHE	A	116	-24.650	-22.627	8.463	1.00	33.88	A
ATOM	881	N	PRO	A	117	-24.425	-20.397	8.238	1.00	36.47	A
ATOM	882	CD	PRO	A	117	-23.799	-19.093	8.500	1.00	37.82	A
ATOM	883	CA	PRO	A	117	-25.260	-20.325	7.042	1.00	38.24	A
ATOM	884	CB	PRO	A	117	-25.299	-18.826	6.721	1.00	38.61	A
ATOM	885	CG	PRO	A	117	-24.854	-18.146	8.000	1.00	38.51	A
ATOM	886	C	PRO	A	117	-24.580	-21.093	5.941	1.00	39.43	A
ATOM	887	O	PRO	A	117	-23.363	-21.079	5.840	1.00	40.03	A
ATOM	888	N	ASN	A	118	-25.366	-21.786	5.133	1.00	41.49	A
ATOM	889	CA	ASN	A	118	-24.818	-22.514	4.005	1.00	42.60	A
ATOM	890	CB	ASN	A	118	-24.654	-23.999	4.334	1.00	45.18	A
ATOM	891	CG	ASN	A	118	-25.954	-24.662	4.699	1.00	46.71	A
ATOM	892	OD1	ASN	A	118	-26.693	-24.180	5.564	1.00	48.14	A
ATOM	893	ND2	ASN	A	118	-26.242	-25.782	4.049	1.00	47.23	A
ATOM	894	C	ASN	A	118	-25.787	-22.308	2.856	1.00	42.69	A
ATOM	895	O	ASN	A	118	-27.006	-32.231	3.065	1.00	43.09	A
ATOM	896	N	LEU	A	119	-25.242	-22.165	1.655	1.00	41.35	A
ATOM	897	CA	LEU	A	119	-26.073	-21.954	0.485	1.00	41.09	A
ATOM	898	CB	LEU	A	119	-25.208	-21.818	-0.774	1.00	38.77	A
ATOM	899	CG	LEU	A	119	-24.451	-20.490	-0.937	1.00	38.25	A
ATOM	900	CD1	LEU	A	119	-23.588	-20.520	-2.192	1.00	37.70	A
ATOM	901	CD2	LEU	A	119	-25.453	-19.357	-1.028	1.00	36.82	A
ATOM	902	C	LEU	A	119	-27.015	-23.132	0.350	1.00	41.13	A
ATOM	903	O	LEU	A	119	-26.623	-24.284	0.577	1.00	41.95	A
ATOM	904	N	ASP	A	120	-28.266	-22.833	0.011	1.00	41.01	A
ATOM	905	CA	ASP	A	120	-29.263	-23.870	-0.171	1.00	41.25	A
ATOM	906	CB	ASP	A	120	-30.624	-23.263	-0.503	1.00	42.92	A
ATOM	907	CG	ASP	A	120	-31.197	-22.481	0.649	1.00	43.98	A
ATOM	908	OD1	ASP	A	120	-31.099	-22.974	1.794	1.00	45.98	A
ATOM	909	OD2	ASP	A	120	-31.745	-21.384	0.411	1.00	45.63	A
ATOM	910	C	ASP	A	120	-28.824	-24.775	-1.302	1.00	40.45	A
ATOM	911	O	ASP	A	120	-28.077	-24.362	-2.197	1.00	40.20	A
ATOM	912	N	ASP	A	121	-29.272	-26.018	-1.253	1.00	38.62	A
ATOM	913	CA	ASP	A	121	-28.919	-26.947	-2.299	1.00	36.77	A
ATOM	914	CB	ASP	A	121	-29.544	-38.319	-2.034	1.00	39.85	A
ATOM	915	CG	ASP	A	121	-28.813	-29.091	-0.944	1.00	43.33	A
ATOM	916	OD1	ASP	A	121	-27.587	-29.317	-1.094	1.00	44.66	A
ATOM	917	OD2	ASP	A	121	-29.460	-29.472	0.059	1.00	45.13	A
ATOM	918	C	ASP	A	121	-29.420	-36.365	-3.614	1.00	33.67	A
ATOM	919	O	ASP	A	121	-30.401	-25.623	-3.656	1.00	33.57	A
ATOM	920	N	TRP	A	122	-28.711	-26.684	-4.681	1.00	30.14	A
ATOM	921	CA	TRP	A	122	-29.077	-26.194	-5.992	1.00	25.84	A
ATOM	922	CB	TRP	A	122	-28.391	-24.839	-6.253	1.00	24.07	A
ATOM	923	CG	TRP	A	122	-26.889	-24.848	-6.119	1.00	21.27	A
ATOM	924	CD2	TRP	A	122	-25.938	-24.939	-7.188	1.00	20.32	A
ATOM	925	CE2	TRP	A	122	-24.654	-24.929	-6.609	1.00	20.70	A
ATOM	926	CE3	TRP	A	122	-26.052	-25.027	-8.580	1.00	17.91	A
ATOM	927	CD1	TRP	A	122	-26.160	-24.786	-4.959	1.00	22.23	A
ATOM	928	NE1	TRP	A	122	-24.817	-24.832	-5.249	1.00	20.82	A
ATOM	929	CZ2	TRP	A	122	-23.486	-25.000	-7.378	1.00	21.15	A
ATOM	930	CZ3	TRP	A	122	-24.899	-25.099	-9.351	1.00	19.53	A
ATOM	931	CH2	TRP	A	122	-23.621	-25.083	-8.743	1.00	19.91	A
ATOM	932	C	TRP	A	122	-28.636	-27.256	-6.992	1.00	25.27	A
ATOM	933	O	TRP	A	122	-28.010	-38.255	-6.618	1.00	24.64	A
ATOM	934	N	GLN	A	123	-28.965	-27.064	-8.257	1.00	22.99	A
ATOM	935	CA	GLN	A	123	-28.612	-28.050	-9.261	1.00	23.31	A
ATOM	936	CB	GLN	A	123	-29.882	-28.686	-9.785	1.00	25.63	A
ATOM	937	CG	GLN	A	123	-29.649	-30.014	-10.410	1.00	31.98	A
ATOM	938	CD	GLN	A	123	-29.414	-31.110	-9.363	1.00	32.90	A
ATOM	939	OE1	GLN	A	123	-28.877	-32.157	-9.681	1.00	36.51	A
ATOM	940	NE2	GLN	A	123	-29.836	-30.869	-8.109	1.00	33.21	A
ATOM	941	C	GLN	A	123	-27.811	-27.488	-10.441	1.00	21.76	A
ATOM	942	O	GLN	A	123	-28.179	-36.467	-10.999	1.00	21.19	A
ATOM	943	N	SER	A	124	-26.743	-28.163	-10.855	1.00	22.29	A
ATOM	944	CA	SER	A	124	-25.993	-27.635	-11.990	1.00	23.13	A
ATOM	945	CB	SER	A	124	-24.548	-28.143	-12.016	1.00	26.37	A
ATOM	946	CG	SER	A	124	-24.479	-29.416	-12.593	1.00	30.20	A
ATOM	947	C	SER	A	124	-26.706	-28.034	-13.274	1.00	22.74	A
ATOM	948	O	SER	A	124	-27.311	-29.119	-13.358	1.00	21.31	A
ATOM	949	N	GLU	A	125	-26.627	-27.150	-14.265	1.00	22.78	A
ATOM	950	CA	GLU	A	125	-27.261	-27.343	-15.553	1.00	23.65	A
ATOM	951	CB	GLU	A	125	-28.368	-26.300	-15.707	1.00	26.17	A
ATOM	952	CG	GLU	A	125	-29.141	-26.116	-14.428	1.00	30.96	A
ATOM	953	CD	GLU	A	125	-30.412	-25.337	-14.617	1.00	34.88	A
ATOM	954	OE1	GLU	A	125	-30.408	-24.412	-15.458	1.00	38.83	A
ATOM	955	OE2	GLU	A	125	-31.409	-25.650	-13.917	1.00	38.64	A
ATOM	956	C	GLU	A	125	-26.274	-27.255	-16.701	1.00	22.71	A
ATOM	957	O	GLU	A	125	-26.561	-27.694	-17.806	1.00	22.51	A
ATOM	958	N	VAL	A	126	-25.101	-26.692	-16.427	1.00	20.09	A
ATOM	959	CA	VAL	A	126	-24.048	-26.531	-17.411	1.00	21.58	A
ATOM	960	CB	VAL	A	126	-24.023	-25.055	-17.937	1.00	22.61	A
ATOM	961	CG1	VAL	A	126	-23.060	-24.927	-19.077	1.00	25.78	A
ATOM	962	CG2	VAL	A	126	-25.433	-24.627	-18.355	1.00	25.22	A
ATOM	963	C	VAL	A	126	-22.730	-26.817	-16.729	1.00	19.60	A
ATOM	964	O	VAL	A	126	-22.476	-26.270	-15.676	1.00	19.58	A
ATOM	965	N	GLU	A	127	-21.898	-27.661	-17.318	1.00	17.89	A

Figure 1 (continued 10)

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ATOM	966	CA	GLU	A	127	-20.602	-27.975	-16.742	1.00	19.23	A
ATOM	967	CB	GLU	A	127	-20.643	-29.341	-16.024	1.00	18.90	A
ATOM	968	CG	GLU	A	127	-21.759	-29.457	-15.033	1.00	18.41	A
ATOM	969	CD	GLU	A	127	-21.797	-30.796	-14.274	1.00	18.10	A
ATOM	970	OE1	GLU	A	127	-21.217	-31.797	-14.742	1.00	22.04	A
ATOM	971	OE2	GLU	A	127	-22.431	-30.819	-13.209	1.00	19.35	A
ATOM	972	C	GLU	A	127	-19.509	-28.013	-17.791	1.00	19.53	A
ATOM	973	O	GLU	A	127	-19.741	-28.464	-18.933	1.00	20.65	A
ATOM	974	N	PHE	A	128	-18.312	-27.578	-17.403	1.00	17.93	A
ATOM	975	CA	PHE	A	128	-17.171	-27.600	-18.304	1.00	18.52	A
ATOM	976	CB	PHE	A	128	-17.329	-26.530	-19.409	1.00	19.39	A
ATOM	977	CG	PHE	A	128	-17.528	-25.136	-18.885	1.00	18.24	A
ATOM	978	CD1	PHE	A	128	-16.423	-24.329	-18.575	1.00	18.53	A
ATOM	979	CD2	PHE	A	128	-18.818	-24.640	-18.668	1.00	18.55	A
ATOM	980	CE1	PHE	A	128	-16.605	-23.031	-18.044	1.00	18.93	A
ATOM	981	CE2	PHE	A	128	-19.014	-23.347	-18.134	1.00	18.45	A
ATOM	982	CZ	PHE	A	128	-17.909	-22.541	-17.822	1.00	17.31	A
ATOM	983	O	PHE	A	128	-15.900	-27.381	-17.519	1.00	19.63	A
ATOM	984	N	PHE	A	128	-15.922	-27.006	-16.335	1.00	16.92	A
ATOM	985	CA	THR	A	129	-14.785	-27.656	-18.174	1.00	19.01	A
ATOM	986	CB	THR	A	129	-13.497	-27.456	-17.561	1.00	21.20	A
ATOM	987	CB	THR	A	129	-12.696	-28.761	-17.436	1.00	24.95	A
ATOM	988	OG1	THR	A	129	-12.403	-29.263	-18.751	1.00	27.82	A
ATOM	989	CG2	THR	A	129	-13.471	-29.800	-16.613	1.00	24.46	A
ATOM	990	C	THR	A	129	-12.729	-26.538	-18.479	1.00	21.52	A
ATOM	991	O	THR	A	129	-13.035	-26.429	-19.669	1.00	24.36	A
ATOM	992	N	LEU	A	130	-11.743	-25.858	-17.923	1.00	21.67	A
ATOM	993	CA	LEU	A	130	-10.885	-25.005	-18.716	1.00	21.43	A
ATOM	994	CB	LEU	A	130	-11.600	-23.722	-19.161	1.00	21.02	A
ATOM	995	CG	LEU	A	130	-11.737	-22.614	-18.130	1.00	21.55	A
ATOM	996	CD1	LEU	A	130	-12.246	-21.359	-18.862	1.00	18.68	A
ATOM	997	CD2	LEU	A	130	-12.684	-23.045	-17.006	1.00	20.37	A
ATOM	998	O	LEU	A	130	-9.666	-24.689	-17.877	1.00	20.77	A
ATOM	999	N	LEU	A	130	-9.676	-24.832	-16.645	1.00	21.88	A
ATOM	1000	O	PRO	A	131	-8.576	-24.302	-18.535	1.00	21.78	A
ATOM	1001	CD	PRO	A	131	-8.433	-24.202	-19.997	1.00	22.11	A
ATOM	1002	CB	PRO	A	131	-7.327	-23.970	-17.864	1.00	22.02	A
ATOM	1003	CG	PRO	A	131	-6.382	-23.669	-19.023	1.00	21.96	A
ATOM	1004	CB	PRO	A	131	-6.975	-24.434	-20.168	1.00	22.46	A
ATOM	1005	O	PRO	A	131	-7.468	-22.772	-16.938	1.00	23.06	A
ATOM	1006	C	PRO	A	131	-8.194	-21.823	-17.256	1.00	22.79	A
ATOM	1007	N	GLN	A	132	-6.767	-22.806	-15.808	1.00	22.91	A
ATOM	1008	CA	GLN	A	132	-6.813	-21.686	-14.868	1.00	23.70	A
ATOM	1009	CB	GLN	A	132	-5.881	-21.922	-13.678	1.00	25.71	A
ATOM	1010	CG	GLN	A	132	-6.311	-23.098	-12.821	1.00	29.70	A
ATOM	1011	CD	GLN	A	132	-5.450	-23.279	-11.576	1.00	32.46	A
ATOM	1012	OE1	GLN	A	132	-5.308	-22.365	-10.762	1.00	32.13	A
ATOM	1013	NE2	GLN	A	132	-4.878	-24.477	-11.425	1.00	33.56	A
ATOM	1014	C	GLN	A	132	-6.394	-20.419	-15.581	1.00	22.79	A
ATOM	1015	O	GLN	A	132	-6.999	-19.368	-15.380	1.00	21.02	A
ATOM	1016	N	ALA	A	133	-5.375	-20.517	-16.424	1.00	21.06	A
ATOM	1017	CA	ALA	A	133	-4.897	-19.337	-17.154	1.00	22.13	A
ATOM	1018	CB	ALA	A	133	-3.624	-19.681	-17.935	1.00	22.47	A
ATOM	1019	C	ALA	A	133	-5.942	-18.757	-18.098	1.00	20.39	A
ATOM	1020	O	ALA	A	133	-5.932	-17.559	-18.361	1.00	21.36	A
ATOM	1021	N	THR	A	134	-6.833	-19.590	-18.630	1.00	18.88	A
ATOM	1022	CA	THR	A	134	-7.853	-19.085	-19.549	1.00	18.20	A
ATOM	1023	CB	THR	A	134	-8.512	-20.254	-20.296	1.00	19.77	A
ATOM	1024	OG1	THR	A	134	-7.498	-20.911	-21.092	1.00	19.04	A
ATOM	1025	CG2	THR	A	134	-9.594	-19.776	-21.214	1.00	18.65	A
ATOM	1026	C	THR	A	134	-8.885	-18.288	-18.773	1.00	17.20	A
ATOM	1027	O	THR	A	134	-9.341	-17.214	-19.190	1.00	16.08	A
ATOM	1028	N	MET	A	135	-9.260	-18.827	-17.627	1.00	17.79	A
ATOM	1029	CA	MET	A	135	-10.237	-18.138	-16.786	1.00	18.34	A
ATOM	1030	CB	MET	A	135	-10.612	-19.011	-15.579	1.00	18.90	A
ATOM	1031	CG	MET	A	135	-11.596	-18.329	-14.623	1.00	21.27	A
ATOM	1032	SD	MET	A	135	-13.215	-17.944	-15.348	1.00	25.97	A
ATOM	1033	CE	MET	A	135	-13.884	-19.343	-15.539	1.00	21.37	A
ATOM	1034	C	MET	A	135	-9.677	-16.800	-16.311	1.00	18.69	A
ATOM	1035	O	MET	A	135	-10.386	-15.793	-16.327	1.00	17.86	A
ATOM	1036	N	LYS	A	136	-8.409	-16.776	-15.890	1.00	18.69	A
ATOM	1037	CA	LYS	A	136	-7.754	-15.553	-15.443	1.00	20.30	A
ATOM	1038	CB	LYS	A	136	-6.302	-15.835	-15.024	1.00	23.59	A
ATOM	1039	CG	LYS	A	136	-5.351	-14.628	-15.146	1.00	28.29	A
ATOM	1040	CD	LYS	A	136	-3.863	-15.004	-14.987	1.00	31.41	A
ATOM	1041	CE	LYS	A	136	-3.406	-16.112	-15.975	1.00	35.30	A
ATOM	1042	NZ	LYS	A	136	-3.714	-15.883	-17.445	1.00	35.62	A
ATOM	1043	C	LYS	A	136	-7.752	-14.531	-16.578	1.00	19.86	A
ATOM	1044	O	LYS	A	136	-8.004	-13.352	-16.364	1.00	20.49	A
ATOM	1045	N	ARG	A	137	-7.445	-14.988	-17.786	1.00	17.95	A
ATOM	1046	CA	ARG	A	137	-7.423	-14.094	-18.915	1.00	16.91	A
ATOM	1047	CB	ARG	A	137	-6.931	-14.844	-20.152	1.00	20.63	A
ATOM	1048	CG	ARG	A	137	-6.418	-13.923	-21.256	1.00	27.85	A
ATOM	1049	CD	ARG	A	137	-7.457	-13.620	-22.307	1.00	32.60	A
ATOM	1050	NE	ARG	A	137	-7.054	-12.470	-23.126	1.00	38.30	A
ATOM	1051	CZ	ARG	A	137	-7.656	-12.105	-24.254	1.00	39.88	A
ATOM	1052	NH1	ARG	A	137	-8.682	-12.806	-24.711	1.00	42.58	A
ATOM	1053	NH2	ARG	A	137	-7.255	-11.029	-24.915	1.00	38.76	A
ATOM	1054	C	ARG	A	137	-8.819	-13.504	-19.171	1.00	16.74	A
ATOM	1055	O	ARG	A	137	-8.950	-12.317	-19.436	1.00	16.26	A
ATOM	1056	N	LEU	A	138	-9.846	-14.333	-19.081	1.00	13.43	A
ATOM	1057	CA	LEU	A	138	-11.202	-13.848	-19.338	1.00	13.64	A
ATOM	1058	CB	LEU	A	138	-12.201	-15.020	-19.290	1.00	14.57	A
ATOM	1059	CG	LEU	A	138	-12.160	-15.924	-20.526	1.00	14.17	A
ATOM	1060	CD1	LEU	A	138	-12.888	-17.223	-20.219	1.00	17.01	A
ATOM	1061	CD2	LEU	A	138	-12.794	-15.194	-21.734	1.00	15.21	A
ATOM	1062	C	LEU	A	138	-11.604	-12.799	-18.341	1.00	13.26	A
ATOM	1063	O	LEU	A	138	-12.232	-11.788	-18.700	1.00	13.04	A
ATOM	1064	N	ILE	A	139	-11.269	-13.036	-17.073	1.00	13.36	A
ATOM	1065	CA	ILE	A	139	-11.642	-12.066	-16.049	1.00	14.01	A

Figure 1 (continued 11)

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ATOM	1066	CB	ILE	A	139	-11.574	-12.711	-14.631	1.00	14.80	A
ATOM	1067	CG2	ILE	A	139	-11.749	-11.612	-13.554	1.00	14.76	A
ATOM	1068	CG1	ILE	A	139	-12.657	-13.793	-14.526	1.00	14.38	A
ATOM	1069	CD1	ILE	A	139	-12.522	-14.700	-13.259	1.00	15.70	A
ATOM	1070	C	ILE	A	139	-10.828	-10.782	-16.115	1.00	15.36	A
ATOM	1071	O	ILE	A	139	-11.403	-9.681	-16.129	1.00	15.94	A
ATOM	1072	N	GLU	A	140	-9.500	-10.891	-16.185	1.00	14.35	A
ATOM	1073	CA	GLU	A	140	-8.663	-9.698	-16.254	1.00	16.18	A
ATOM	1074	CB	GLU	A	140	-7.175	-10.107	-16.250	1.00	18.11	A
ATOM	1075	CG	GLU	A	140	-6.708	-10.696	-14.927	1.00	24.32	A
ATOM	1076	CD	GLU	A	140	-5.209	-11.032	-14.909	1.00	29.34	A
ATOM	1077	OE1	GLU	A	140	-4.642	-11.276	-15.995	1.00	31.06	A
ATOM	1078	OE2	GLU	A	140	-4.606	-11.069	-13.804	1.00	33.19	A
ATOM	1079	C	GLU	A	140	-8.955	-8.832	-17.481	1.00	15.66	A
ATOM	1080	O	GLU	A	140	-8.774	-7.613	-17.452	1.00	16.06	A
ATOM	1081	N	ALA	A	141	-9.428	-9.458	-18.547	1.00	14.10	A
ATOM	1082	CA	ALA	A	141	-9.690	-8.725	-19.785	1.00	12.46	A
ATOM	1083	CB	ALA	A	141	-9.921	-9.712	-20.945	1.00	16.01	A
ATOM	1084	C	ALA	A	141	-10.893	-7.796	-19.666	1.00	13.15	A
ATOM	1085	O	ALA	A	141	-11.005	-6.834	-20.422	1.00	12.75	A
ATOM	1086	N	THR	A	142	-11.771	-8.088	-18.726	1.00	12.50	A
ATOM	1087	CA	THR	A	142	-13.017	-7.313	-18.635	1.00	10.74	A
ATOM	1088	CB	THR	A	142	-14.234	-8.165	-19.093	1.00	11.13	A
ATOM	1089	CG1	THR	A	142	-14.408	-9.249	-18.173	1.00	15.23	A
ATOM	1090	CG2	THR	A	142	-14.000	-8.750	-20.499	1.00	11.74	A
ATOM	1091	C	THR	A	142	-13.397	-6.766	-17.277	1.00	13.68	A
ATOM	1092	O	THR	A	142	-14.208	-5.849	-17.229	1.00	12.84	A
ATOM	1093	N	GLN	A	143	-12.824	-7.279	-16.193	1.00	12.98	A
ATOM	1094	CA	GLN	A	143	-13.218	-6.886	-14.832	1.00	14.94	A
ATOM	1095	CB	GLN	A	143	-12.264	-7.548	-13.841	1.00	17.55	A
ATOM	1096	CG	GLN	A	143	-12.686	-7.401	-12.422	1.00	23.99	A
ATOM	1097	CD	GLN	A	143	-11.760	-8.145	-11.481	1.00	27.58	A
ATOM	1098	OE1	GLN	A	143	-12.121	-8.446	-10.332	1.00	31.11	A
ATOM	1099	NE2	GLN	A	143	-10.561	-8.434	-11.956	1.00	27.03	A
ATOM	1100	C	GLN	A	143	-13.311	-5.398	-14.533	1.00	14.23	A
ATOM	1101	O	GLN	A	143	-14.235	-4.946	-13.808	1.00	15.54	A
ATOM	1102	N	PHE	A	144	-12.372	-4.641	-15.073	1.00	14.47	A
ATOM	1103	CA	PHE	A	144	-12.312	-3.206	-14.848	1.00	14.06	A
ATOM	1104	CB	PHE	A	144	-11.028	-2.636	-15.430	1.00	13.76	A
ATOM	1105	CG	PHE	A	144	-11.014	-2.621	-16.924	1.00	16.11	A
ATOM	1106	CD1	PHE	A	144	-10.537	-3.718	-17.656	1.00	14.91	A
ATOM	1107	CD2	PHE	A	144	-11.524	-1.510	-17.611	1.00	15.82	A
ATOM	1108	OE1	PHE	A	144	-10.567	-2.701	-19.064	1.00	15.95	A
ATOM	1109	OE2	PHE	A	144	-11.558	-1.484	-19.000	1.00	16.83	A
ATOM	1110	C	PHE	A	144	-11.080	-2.579	-19.730	1.00	18.10	A
ATOM	1111	O	PHE	A	144	-13.503	-2.424	-15.388	1.00	15.25	A
ATOM	1112	N	SER	A	145	-13.727	-1.296	-14.957	1.00	14.82	A
ATOM	1113	CA	SER	A	145	-14.268	-3.019	-16.306	1.00	13.80	A
ATOM	1114	CB	SER	A	145	-15.442	-2.334	-16.873	1.00	14.34	A
ATOM	1115	CG	SER	A	145	-15.637	-2.720	-18.328	1.00	15.77	A
ATOM	1116	CD	SER	A	145	-14.570	-2.200	-19.120	1.00	16.45	A
ATOM	1117	O	SER	A	145	-16.737	-2.587	-16.121	1.00	15.00	A
ATOM	1118	N	SER	A	145	-17.787	-2.069	-16.526	1.00	15.49	A
ATOM	1119	C	MET	A	146	-16.699	-3.407	-15.084	1.00	15.16	A
ATOM	1120	CA	MET	A	146	-17.917	-3.660	-14.288	1.00	15.61	A
ATOM	1121	CB	MET	A	146	-17.677	-4.746	-13.224	1.00	16.31	A
ATOM	1122	CG	MET	A	146	-17.414	-6.142	-13.771	1.00	16.90	A
ATOM	1123	CD	MET	A	146	-17.264	-7.426	-12.423	1.00	20.35	A
ATOM	1124	CE	MET	A	146	-15.868	-6.822	-11.667	1.00	18.34	A
ATOM	1125	C	MET	A	146	-18.290	-2.364	-13.546	1.00	17.87	A
ATOM	1126	O	MET	A	146	-17.436	-1.571	-13.177	1.00	17.71	A
ATOM	1127	N	ALA	A	147	-19.584	-2.171	-13.302	1.00	18.85	A
ATOM	1128	CA	ALA	A	147	-20.000	-0.987	-12.561	1.00	22.61	A
ATOM	1129	CB	ALA	A	147	-21.514	-0.786	-12.718	1.00	20.80	A
ATOM	1130	C	ALA	A	147	-19.666	-1.181	-11.088	1.00	25.26	A
ATOM	1131	O	ALA	A	147	-19.455	-2.315	-10.624	1.00	25.14	A
ATOM	1132	N	HIS	A	148	-19.654	-0.068	-10.359	1.00	29.57	A
ATOM	1133	CA	HIS	A	148	-19.407	-0.078	-8.916	1.00	32.55	A
ATOM	1134	CB	HIS	A	148	-18.185	0.755	-8.530	1.00	35.09	A
ATOM	1135	CG	HIS	A	148	-16.886	0.218	-9.025	1.00	38.05	A
ATOM	1136	CD	HIS	A	148	-15.868	-0.390	-8.368	1.00	38.84	A
ATOM	1137	ND1	HIS	A	148	-16.477	0.347	-10.336	1.00	39.33	A
ATOM	1138	CE1	HIS	A	148	-15.259	-0.151	-10.463	1.00	39.25	A
ATOM	1139	NE2	HIS	A	148	-14.867	-0.603	-9.284	1.00	39.69	A
ATOM	1140	C	HIS	A	148	-20.588	0.578	-8.210	1.00	32.61	A
ATOM	1141	O	HIS	A	148	-20.810	1.781	-8.365	1.00	33.21	A
ATOM	1142	N	GLN	A	149	-21.326	-0.203	-7.436	1.00	32.56	A
ATOM	1143	CA	GLN	A	149	-22.449	0.309	-6.663	1.00	33.37	A
ATOM	1144	CB	GLN	A	149	-21.922	1.256	-5.575	1.00	35.74	A
ATOM	1145	CG	GLN	A	149	-20.875	0.614	-4.657	1.00	39.57	A
ATOM	1146	CD	GLN	A	149	-20.358	1.564	-3.573	1.00	41.69	A
ATOM	1147	OE1	GLN	A	149	-21.099	2.399	-3.059	1.00	42.95	A
ATOM	1148	NE2	GLN	A	149	-19.084	1.420	-3.214	1.00	41.85	A
ATOM	1149	C	GLN	A	149	-23.529	1.008	-7.486	1.00	32.00	A
ATOM	1150	O	GLN	A	149	-24.177	1.957	-7.016	1.00	32.50	A
ATOM	1151	N	ASP	A	150	-23.742	0.538	-8.704	1.00	29.36	A
ATOM	1152	CA	ASP	A	150	-24.772	1.110	-9.560	1.00	27.85	A
ATOM	1153	CB	ASP	A	150	-24.532	0.681	-11.006	1.00	26.70	A
ATOM	1154	CG	ASP	A	150	-25.318	1.510	-12.007	1.00	27.39	A
ATOM	1155	OD1	ASP	A	150	-24.695	2.262	-12.791	1.00	27.00	A
ATOM	1156	OD2	ASP	A	150	-26.558	1.410	-12.017	1.00	26.08	A
ATOM	1157	C	ASP	A	150	-26.143	0.601	-9.093	1.00	27.65	A
ATOM	1158	O	ASP	A	150	-26.291	-0.565	-8.720	1.00	27.65	A
ATOM	1159	N	VAL	A	151	-27.148	1.475	-9.100	1.00	28.95	A
ATOM	1160	CA	VAL	A	151	-28.495	1.080	-8.702	1.00	30.15	A
ATOM	1161	CB	VAL	A	151	-29.462	2.274	-8.840	1.00	30.10	A
ATOM	1162	CG1	VAL	A	151	-30.898	1.825	-8.593	1.00	33.02	A
ATOM	1163	CG2	VAL	A	151	-29.065	3.354	-7.856	1.00	32.71	A
ATOM	1164	C	VAL	A	151	-28.985	-0.099	-9.552	1.00	29.78	A
ATOM	1165	O	VAL	A	151	-29.860	-0.858	-9.137	1.00	29.45	A

Figure 1 (continued 12)

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ATOM	1166	N	ARG	A	152	-28.431	-0.251	-10.752	1.00	29.05	A
ATOM	1167	CA	ARG	A	152	-28.804	-1.379	-11.596	1.00	27.89	A
ATOM	1168	CB	ARG	A	152	-28.634	-1.019	-13.069	1.00	26.83	A
ATOM	1169	CG	ARG	A	152	-29.512	0.180	-13.508	1.00	26.45	A
ATOM	1170	CD	ARG	A	152	-29.040	0.760	-14.836	1.00	26.01	A
ATOM	1171	NE	ARG	A	152	-27.778	1.484	-14.686	1.00	24.71	A
ATOM	1172	CZ	ARG	A	152	-27.089	2.005	-15.701	1.00	21.61	A
ATOM	1173	NH1	ARG	A	152	-27.529	1.890	-16.950	1.00	23.37	A
ATOM	1174	NH2	ARG	A	152	-25.947	2.627	-15.469	1.00	22.47	A
ATOM	1175	C	ARG	A	152	-27.813	-2.455	-11.176	1.00	27.21	A
ATOM	1176	O	ARG	A	152	-26.719	-2.545	-11.722	1.00	24.79	A
ATOM	1177	N	TYR	A	153	-28.197	-3.226	-10.163	1.00	27.89	A
ATOM	1178	CA	TYR	A	153	-27.379	-4.284	-9.588	1.00	28.26	A
ATOM	1179	CB	TYR	A	153	-28.198	-5.074	-8.566	1.00	32.74	A
ATOM	1180	CG	TYR	A	153	-29.435	-5.685	-9.190	1.00	36.87	A
ATOM	1181	CD1	TYR	A	153	-30.400	-4.879	-9.808	1.00	39.09	A
ATOM	1182	CE1	TYR	A	153	-31.510	-5.434	-10.445	1.00	41.32	A
ATOM	1183	CD2	TYR	A	153	-29.620	-7.069	-9.212	1.00	38.75	A
ATOM	1184	CE2	TYR	A	153	-30.734	-7.637	-9.839	1.00	41.39	A
ATOM	1185	CZ	TYR	A	153	-31.670	-6.814	-10.459	1.00	41.82	A
ATOM	1186	OH	TYR	A	153	-32.744	-7.366	-11.122	1.00	43.97	A
ATOM	1187	C	TYR	A	153	-26.802	-5.265	-10.594	1.00	25.95	A
ATOM	1188	O	TYR	A	153	-25.720	-5.798	-10.355	1.00	25.41	A
ATOM	1189	N	TYR	A	154	-27.521	-5.522	-11.683	1.00	24.27	A
ATOM	1190	CA	TYR	A	154	-27.038	-6.478	-12.683	1.00	24.02	A
ATOM	1191	CB	TYR	A	154	-28.138	-6.822	-13.697	1.00	24.80	A
ATOM	1192	CG	TYR	A	154	-28.704	-5.632	-14.441	1.00	26.56	A
ATOM	1193	CD1	TYR	A	154	-28.095	-5.150	-15.603	1.00	26.67	A
ATOM	1194	CE1	TYR	A	154	-28.609	-4.046	-16.280	1.00	28.56	A
ATOM	1195	CD2	TYR	A	154	-29.841	-4.982	-13.969	1.00	27.71	A
ATOM	1196	CE2	TYR	A	154	-30.366	-3.868	-14.636	1.00	28.26	A
ATOM	1197	CZ	TYR	A	154	-29.745	-3.411	-15.789	1.00	29.38	A
ATOM	1198	OH	TYR	A	154	-30.269	-2.332	-16.463	1.00	31.98	A
ATOM	1199	C	TYR	A	154	-25.786	-5.988	-13.410	1.00	23.05	A
ATOM	1200	O	TYR	A	154	-25.156	-6.778	-14.135	1.00	24.65	A
ATOM	1201	N	LEU	A	155	-25.433	-4.709	-13.249	1.00	19.62	A
ATOM	1202	CA	LEU	A	155	-24.215	-4.190	-13.884	1.00	18.55	A
ATOM	1203	CB	LEU	A	155	-24.397	-2.720	-14.330	1.00	18.29	A
ATOM	1204	CG	LEU	A	155	-25.393	-2.508	-15.470	1.00	18.19	A
ATOM	1205	CD1	LEU	A	155	-25.430	-1.025	-15.872	1.00	20.01	A
ATOM	1206	CD2	LEU	A	155	-24.986	-3.351	-16.652	1.00	17.70	A
ATOM	1207	C	LEU	A	155	-23.029	-4.270	-12.926	1.00	18.16	A
ATOM	1208	O	LEU	A	155	-21.890	-4.047	-13.335	1.00	17.47	A
ATOM	1209	N	ASN	A	156	-23.299	-4.538	-11.648	1.00	19.44	A
ATOM	1210	CA	ASN	A	156	-22.258	-4.646	-10.622	1.00	19.29	A
ATOM	1211	CB	ASN	A	156	-22.776	-4.318	-9.225	1.00	20.80	A
ATOM	1212	CG	ASN	A	156	-23.318	-2.927	-9.107	1.00	21.25	A
ATOM	1213	OD1	ASN	A	156	-24.221	-2.673	-8.287	1.00	24.83	A
ATOM	1214	ND2	ASN	A	156	-22.777	-2.010	-9.887	1.00	16.70	A
ATOM	1215	C	ASN	A	156	-21.821	-6.113	-10.587	1.00	19.89	A
ATOM	1216	O	ASN	A	156	-21.828	-6.805	-9.535	1.00	23.37	A
ATOM	1217	N	GLY	A	157	-21.518	-6.613	-11.753	1.00	17.85	A
ATOM	1218	CA	GLY	A	157	-21.070	-7.981	-11.823	1.00	16.12	A
ATOM	1219	C	GLY	A	157	-20.565	-8.215	-13.217	1.00	14.85	A
ATOM	1220	O	GLY	A	157	-20.399	-7.275	-13.993	1.00	15.61	A
ATOM	1221	N	MET	A	158	-20.343	-9.485	-13.544	1.00	13.48	A
ATOM	1222	CA	MET	A	158	-19.800	-9.852	-14.842	1.00	13.97	A
ATOM	1223	CB	MET	A	158	-18.349	-10.347	-14.646	1.00	13.51	A
ATOM	1224	CG	MET	A	158	-17.648	-10.766	-15.928	1.00	12.71	A
ATOM	1225	SD	MET	A	158	-15.937	-11.277	-15.551	1.00	12.75	A
ATOM	1226	CE	MET	A	158	-15.144	-9.642	-15.273	1.00	14.07	A
ATOM	1227	C	MET	A	158	-20.622	-10.936	-15.511	1.00	12.85	A
ATOM	1228	O	MET	A	158	-20.950	-11.942	-14.890	1.00	12.99	A
ATOM	1229	N	LEU	A	159	-20.941	-10.757	-16.787	1.00	11.15	A
ATOM	1230	CA	LEU	A	159	-21.692	-11.772	-17.517	1.00	12.65	A
ATOM	1231	CB	LEU	A	159	-22.302	-11.197	-18.799	1.00	14.78	A
ATOM	1232	CG	LEU	A	159	-23.251	-12.145	-19.553	1.00	16.09	A
ATOM	1233	CD1	LEU	A	159	-24.545	-12.193	-18.732	1.00	16.30	A
ATOM	1234	CD2	LEU	A	159	-23.582	-11.680	-20.975	1.00	17.74	A
ATOM	1235	C	LEU	A	159	-20.737	-12.884	-17.923	1.00	13.59	A
ATOM	1236	O	LEU	A	159	-19.642	-12.598	-18.386	1.00	12.32	A
ATOM	1237	N	PHE	A	160	-21.138	-14.119	-17.652	1.00	13.23	A
ATOM	1238	CA	PHE	A	160	-20.369	-15.298	-18.110	1.00	13.78	A
ATOM	1239	CB	PHE	A	160	-20.017	-16.243	-16.972	1.00	15.17	A
ATOM	1240	CG	PHE	A	160	-18.810	-15.822	-16.206	1.00	15.50	A
ATOM	1241	CD1	PHE	A	160	-18.845	-14.708	-15.386	1.00	16.70	A
ATOM	1242	CD2	PHE	A	160	-17.619	-16.528	-16.340	1.00	20.57	A
ATOM	1243	CE1	PHE	A	160	-17.690	-14.301	-14.696	1.00	15.09	A
ATOM	1244	CE2	PHE	A	160	-16.473	-16.129	-15.664	1.00	21.51	A
ATOM	1245	CZ	PHE	A	160	-16.516	-15.010	-14.837	1.00	19.20	A
ATOM	1246	O	PHE	A	160	-21.324	-15.985	-19.078	1.00	14.91	A
ATOM	1247	N	PHE	A	160	-22.457	-16.356	-18.712	1.00	14.88	A
ATOM	1248	C	GLU	A	161	-20.883	-16.155	-20.326	1.00	14.48	A
ATOM	1249	CA	GLU	A	161	-21.732	-16.732	-21.343	1.00	15.81	A
ATOM	1250	CB	GLU	A	161	-22.136	-15.629	-22.347	1.00	17.40	A
ATOM	1251	CG	GLU	A	161	-22.921	-15.096	-23.576	1.00	21.36	A
ATOM	1252	CD	GLU	A	161	-23.306	-14.959	-24.539	1.00	25.94	A
ATOM	1253	OE1	GLU	A	161	-22.630	-13.893	-24.551	1.00	23.68	A
ATOM	1254	OE2	GLU	A	161	-24.296	-15.148	-25.306	1.00	27.60	A
ATOM	1255	C	GLU	A	161	-21.042	-17.858	-22.070	1.00	16.27	A
ATOM	1256	O	GLU	A	161	-19.852	-17.753	-22.420	1.00	16.32	A
ATOM	1257	N	THR	A	162	-21.785	-18.939	-22.275	1.00	16.15	A
ATOM	1258	CA	THR	A	162	-21.255	-20.072	-23.043	1.00	17.00	A
ATOM	1259	CB	THR	A	162	-21.579	-21.416	-22.376	1.00	15.79	A
ATOM	1260	OG1	THR	A	162	-22.976	-21.471	-22.079	1.00	17.17	A
ATOM	1261	OG2	THR	A	162	-20.777	-21.587	-21.073	1.00	17.18	A
ATOM	1262	C	THR	A	162	-21.943	-20.022	-24.408	1.00	16.86	A
ATOM	1263	O	THR	A	162	-23.133	-19.814	-24.498	1.00	17.96	A
ATOM	1264	N	GLU	A	163	-21.184	-20.213	-25.473	1.00	19.48	A
ATOM	1265	CA	GLU	A	163	-21.770	-20.170	-26.807	1.00	20.26	A

Figure 1 (continued 13)

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ATOM	1266	CB	GLU	A	163	-21.892	-18.717	-27.287	1.00	21.73	A
ATOM	1267	CG	GLU	A	163	-22.630	-18.615	-28.630	1.00	25.04	A
ATOM	1268	CD	GLU	A	163	-22.892	-17.188	-29.043	1.00	28.71	A
ATOM	1269	OE1	GLU	A	163	-22.046	-16.326	-28.755	1.00	29.00	A
ATOM	1270	OE2	GLU	A	163	-23.937	-16.925	-29.672	1.00	33.20	A
ATOM	1271	C	GLU	A	163	-20.857	-20.965	-27.717	1.00	20.58	A
ATOM	1272	O	GLU	A	163	-19.670	-20.671	-27.849	1.00	19.51	A
ATOM	1273	N	GLY	A	164	-21.427	-21.985	-28.336	1.00	21.25	A
ATOM	1274	CA	GLY	A	164	-20.643	-22.834	-29.208	1.00	23.06	A
ATOM	1275	C	GLY	A	164	-19.570	-23.516	-28.381	1.00	22.55	A
ATOM	1276	O	GLY	A	164	-19.860	-24.269	-27.441	1.00	23.22	A
ATOM	1277	N	GLU	A	165	-18.323	-23.232	-28.699	1.00	22.46	A
ATOM	1278	CA	GLU	A	165	-17.233	-23.835	-27.965	1.00	21.86	A
ATOM	1279	CB	GLU	A	165	-16.276	-24.498	-28.948	1.00	26.05	A
ATOM	1280	CG	GLU	A	165	-15.133	-25.183	-28.299	1.00	31.89	A
ATOM	1281	CD	GLU	A	165	-13.996	-25.386	-29.268	1.00	32.82	A
ATOM	1282	OE1	GLU	A	165	-14.228	-26.054	-30.316	1.00	35.85	A
ATOM	1283	OE2	GLU	A	165	-12.891	-24.872	-28.983	1.00	32.38	A
ATOM	1284	C	GLU	A	165	-16.492	-22.792	-27.122	1.00	20.54	A
ATOM	1285	O	GLU	A	165	-15.403	-23.031	-26.629	1.00	21.57	A
ATOM	1286	N	GLU	A	166	-17.101	-21.632	-26.932	1.00	18.84	A
ATOM	1287	CA	GLU	A	166	-16.419	-20.588	-26.183	1.00	18.69	A
ATOM	1288	CB	GLU	A	166	-16.291	-19.332	-27.036	1.00	20.53	A
ATOM	1289	CG	GLU	A	166	-15.371	-19.476	-28.244	1.00	25.65	A
ATOM	1290	CD	GLU	A	166	-15.124	-18.128	-28.875	1.00	29.36	A
ATOM	1291	OE1	GLU	A	166	-16.106	-17.495	-29.317	1.00	29.76	A
ATOM	1292	OE2	GLU	A	166	-13.953	-17.697	-28.911	1.00	32.95	A
ATOM	1293	C	GLU	A	166	-17.075	-20.149	-24.882	1.00	16.09	A
ATOM	1294	O	GLU	A	166	-18.281	-20.299	-24.699	1.00	17.27	A
ATOM	1295	N	LEU	A	167	-16.226	-19.667	-23.984	1.00	16.29	A
ATOM	1296	CA	LEU	A	167	-16.685	-19.074	-22.722	1.00	14.08	A
ATOM	1297	CB	LEU	A	167	-15.916	-19.586	-21.510	1.00	14.28	A
ATOM	1298	CG	LEU	A	167	-16.345	-18.898	-20.199	1.00	14.34	A
ATOM	1299	CD1	LEU	A	167	-17.852	-19.118	-19.991	1.00	15.20	A
ATOM	1300	CD2	LEU	A	167	-15.572	-19.425	-18.995	1.00	15.60	A
ATOM	1301	C	LEU	A	167	-16.356	-17.589	-22.956	1.00	14.38	A
ATOM	1302	O	LEU	A	167	-15.249	-17.243	-23.413	1.00	14.90	A
ATOM	1303	N	ARG	A	168	-17.314	-16.720	-22.632	1.00	13.15	A
ATOM	1304	CA	ARG	A	168	-17.142	-15.283	-22.858	1.00	13.65	A
ATOM	1305	CB	ARG	A	168	-18.109	-14.851	-23.974	1.00	14.89	A
ATOM	1306	CG	ARG	A	168	-18.286	-13.333	-24.147	1.00	14.54	A
ATOM	1307	CD	ARG	A	168	-19.316	-13.059	-25.217	1.00	16.30	A
ATOM	1308	NE	ARG	A	168	-18.918	-13.676	-26.473	1.00	19.44	A
ATOM	1309	CZ	ARG	A	168	-19.627	-14.584	-27.139	1.00	21.39	A
ATOM	1310	NH1	ARG	A	168	-20.793	-15.006	-26.690	1.00	22.67	A
ATOM	1311	NH2	ARG	A	168	-19.147	-15.073	-28.265	1.00	25.38	A
ATOM	1312	C	ARG	A	168	-17.509	-14.523	-21.605	1.00	13.95	A
ATOM	1313	O	ARG	A	168	-18.425	-14.932	-20.873	1.00	14.10	A
ATOM	1314	N	THR	A	169	-16.794	-13.431	-21.351	1.00	12.43	A
ATOM	1315	CA	THR	A	169	-17.153	-12.587	-20.230	1.00	10.45	A
ATOM	1316	CB	THR	A	169	-16.053	-12.425	-19.186	1.00	12.78	A
ATOM	1317	CG1	THR	A	169	-14.844	-11.981	-19.830	1.00	14.14	A
ATOM	1318	CG2	THR	A	169	-15.808	-13.743	-18.422	1.00	11.68	A
ATOM	1319	C	THR	A	169	-17.469	-11.219	-20.825	1.00	11.09	A
ATOM	1320	O	THR	A	169	-16.932	-10.824	-21.853	1.00	10.97	A
ATOM	1321	N	VAL	A	170	-18.421	-10.537	-20.198	1.00	10.12	A
ATOM	1322	CA	VAL	A	170	-18.803	-9.205	-20.645	1.00	10.95	A
ATOM	1323	CB	VAL	A	170	-20.166	-9.186	-21.384	1.00	10.17	A
ATOM	1324	CG1	VAL	A	170	-20.344	-7.769	-22.015	1.00	11.54	A
ATOM	1325	CG2	VAL	A	170	-20.197	-10.227	-22.491	1.00	13.32	A
ATOM	1326	C	VAL	A	170	-18.967	-8.359	-19.376	1.00	10.18	A
ATOM	1327	O	VAL	A	170	-19.500	-8.824	-18.361	1.00	13.17	A
ATOM	1328	N	ALA	A	171	-18.471	-7.118	-19.426	1.00	11.08	A
ATOM	1329	CA	ALA	A	171	-18.650	-6.212	-18.310	1.00	10.99	A
ATOM	1330	CB	ALA	A	171	-17.451	-6.224	-17.401	1.00	12.41	A
ATOM	1331	C	ALA	A	171	-18.898	-4.807	-18.854	1.00	12.83	A
ATOM	1332	O	ALA	A	171	-18.353	-4.409	-19.875	1.00	13.33	A
ATOM	1333	N	THR	A	172	-19.788	-4.091	-18.193	1.00	11.14	A
ATOM	1334	CA	THR	A	172	-20.092	-2.723	-18.627	1.00	12.97	A
ATOM	1335	CB	THR	A	172	-21.046	-2.669	-19.850	1.00	16.11	A
ATOM	1336	OG1	THR	A	172	-21.222	-1.284	-20.236	1.00	15.65	A
ATOM	1337	CG2	THR	A	172	-22.435	-3.271	-19.520	1.00	15.53	A
ATOM	1338	C	THR	A	172	-20.697	-1.934	-17.486	1.00	13.38	A
ATOM	1339	O	THR	A	172	-21.347	-2.484	-16.592	1.00	13.88	A
ATOM	1340	N	ASP	A	173	-20.455	-0.624	-17.525	1.00	13.39	A
ATOM	1341	CA	ASP	A	173	-20.994	0.264	-16.494	1.00	15.62	A
ATOM	1342	CB	ASP	A	173	-19.864	0.956	-15.731	1.00	16.03	A
ATOM	1343	CG	ASP	A	173	-18.990	1.833	-16.625	1.00	16.32	A
ATOM	1344	OD1	ASP	A	173	-19.273	1.986	-17.831	1.00	15.70	A
ATOM	1345	OD2	ASP	A	173	-18.005	2.370	-16.079	1.00	18.84	A
ATOM	1346	C	ASP	A	173	-21.867	1.310	-17.164	1.00	16.64	A
ATOM	1347	O	ASP	A	173	-22.214	2.322	-16.530	1.00	19.53	A
ATOM	1348	N	GLY	A	174	-22.187	1.083	-18.436	1.00	16.21	A
ATOM	1349	CA	GLY	A	174	-23.039	2.014	-19.178	1.00	18.97	A
ATOM	1350	C	GLY	A	174	-22.302	3.071	-19.977	1.00	19.77	A
ATOM	1351	O	GLY	A	174	-22.884	3.728	-20.860	1.00	21.66	A
ATOM	1352	N	HIS	A	175	-21.023	3.258	-19.655	1.00	18.37	A
ATOM	1353	CA	HIS	A	175	-20.162	4.210	-20.370	1.00	19.07	A
ATOM	1354	CB	HIS	A	175	-19.434	5.082	-19.384	1.00	21.34	A
ATOM	1355	CG	HIS	A	175	-20.339	5.944	-18.578	1.00	28.96	A
ATOM	1356	CD2	HIS	A	175	-20.783	5.827	-17.305	1.00	31.83	A
ATOM	1357	ND1	HIS	A	175	-21.007	7.617	-19.126	1.00	31.01	A
ATOM	1358	CE1	HIS	A	175	-21.828	7.524	-18.225	1.00	30.90	A
ATOM	1359	NE2	HIS	A	175	-21.713	6.820	-17.111	1.00	34.27	A
ATOM	1360	C	HIS	A	175	-19.189	3.501	-21.254	1.00	17.40	A
ATOM	1361	O	HIS	A	175	-18.861	3.970	-22.340	1.00	18.83	A
ATOM	1362	N	ARG	A	176	-18.663	2.385	-20.755	1.00	15.38	A
ATOM	1363	CA	ARG	A	176	-17.713	1.611	-21.529	1.00	14.12	A
ATOM	1364	CB	ARG	A	176	-16.248	1.967	-21.167	1.00	14.64	A
ATOM	1365	CG	ARG	A	176	-15.987	2.385	-19.734	1.00	15.67	A

Figure 1 (continued 14)

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ATOM	1366	CD	ARG	A	176	-15.877	1.156	-18.816	1.00	15.21	A
ATOM	1367	NE	ARG	A	176	-15.566	1.544	-17.439	1.00	14.17	A
ATOM	1368	CZ	ARG	A	176	-14.353	1.799	-16.937	1.00	16.17	A
ATOM	1369	NH1	ARG	A	176	-13.264	1.720	-17.703	1.00	14.70	A
ATOM	1370	NH2	ARG	A	176	-14.223	2.102	-15.644	1.00	16.59	A
ATOM	1371	C	ARG	A	176	-18.026	0.146	-21.304	1.00	12.49	A
ATOM	1372	O	ARG	A	176	-18.629	-0.217	-20.280	1.00	13.08	A
ATOM	1373	N	LEU	A	177	-17.628	-0.684	-22.262	1.00	11.81	A
ATOM	1374	CA	LEU	A	177	-17.922	-2.105	-22.203	1.00	10.41	A
ATOM	1375	CB	LEU	A	177	-19.100	-2.440	-23.151	1.00	11.88	A
ATOM	1376	CG	LEU	A	177	-19.466	-3.935	-23.318	1.00	10.26	A
ATOM	1377	CG1	LEU	A	177	-20.967	-4.089	-23.579	1.00	13.42	A
ATOM	1378	CG2	LEU	A	177	-18.693	-4.547	-24.453	1.00	12.11	A
ATOM	1379	O	LEU	A	177	-16.685	-2.882	-22.630	1.00	11.58	A
ATOM	1380	O	LEU	A	177	-15.896	-2.415	-23.455	1.00	12.23	A
ATOM	1381	N	ALA	A	178	-16.524	-4.055	-22.029	1.00	10.67	A
ATOM	1382	CA	ALA	A	178	-15.417	-4.939	-22.349	1.00	11.62	A
ATOM	1383	CB	ALA	A	178	-14.417	-5.005	-21.178	1.00	11.64	A
ATOM	1384	CG	ALA	A	178	-15.972	-6.330	-22.617	1.00	12.71	A
ATOM	1385	O	ALA	A	178	-16.842	-6.774	-21.876	1.00	12.95	A
ATOM	1386	N	VAL	A	179	-15.510	-7.003	-23.678	1.00	12.86	A
ATOM	1387	CA	VAL	A	179	-15.960	-8.374	-23.931	1.00	11.78	A
ATOM	1388	CB	VAL	A	179	-17.058	-8.434	-25.021	1.00	13.43	A
ATOM	1389	CG1	VAL	A	179	-16.623	-7.680	-26.291	1.00	13.32	A
ATOM	1390	CG2	VAL	A	179	-17.401	-9.905	-25.341	1.00	13.70	A
ATOM	1391	C	VAL	A	179	-14.771	-9.221	-24.330	1.00	12.02	A
ATOM	1392	O	VAL	A	179	-13.897	-8.750	-25.047	1.00	13.44	A
ATOM	1393	N	CYS	A	180	-14.736	-10.463	-23.853	1.00	11.67	A
ATOM	1394	CA	CYS	A	180	-13.611	-11.330	-24.205	1.00	12.63	A
ATOM	1395	CB	CYS	A	180	-12.567	-11.260	-23.107	1.00	12.65	A
ATOM	1396	SG	CYS	A	180	-11.064	-12.239	-23.457	1.00	16.29	A
ATOM	1397	C	CYS	A	180	-14.123	-12.752	-24.329	1.00	14.48	A
ATOM	1398	O	CYS	A	180	-14.900	-13.187	-23.487	1.00	14.59	A
ATOM	1399	N	SER	A	181	-13.722	-13.467	-25.379	1.00	14.95	A
ATOM	1400	CA	SER	A	181	-14.178	-14.859	-25.516	1.00	17.59	A
ATOM	1401	CB	SER	A	181	-15.229	-15.019	-26.640	1.00	20.93	A
ATOM	1402	CG	SER	A	181	-14.687	-14.808	-27.912	1.00	26.78	A
ATOM	1403	C	SER	A	181	-12.970	-15.726	-25.794	1.00	17.42	A
ATOM	1404	O	SER	A	181	-12.009	-15.274	-26.428	1.00	18.86	A
ATOM	1405	N	MET	A	182	-13.020	-16.953	-25.305	1.00	16.52	A
ATOM	1406	CA	MET	A	182	-11.929	-17.925	-25.453	1.00	17.26	A
ATOM	1407	CB	MET	A	182	-11.075	-17.953	-24.177	1.00	20.28	A
ATOM	1408	CG	MET	A	182	-10.358	-16.670	-23.853	1.00	22.98	A
ATOM	1409	SD	MET	A	182	-8.999	-16.391	-24.945	1.00	26.97	A
ATOM	1410	CE	MET	A	182	-7.745	-17.563	-24.206	1.00	26.51	A
ATOM	1411	C	MET	A	182	-12.489	-19.310	-25.681	1.00	18.28	A
ATOM	1412	O	MET	A	182	-13.421	-19.734	-25.022	1.00	17.56	A
ATOM	1413	N	PRO	A	183	-11.906	-20.056	-26.629	1.00	19.27	A
ATOM	1414	CA	PRO	A	183	-10.796	-19.620	-27.496	1.00	19.63	A
ATOM	1415	CB	PRO	A	183	-12.345	-21.411	-26.955	1.00	20.53	A
ATOM	1416	CG	PRO	A	183	-11.645	-21.677	-28.300	1.00	21.37	A
ATOM	1417	O	PRO	A	183	-10.352	-20.944	-28.145	1.00	21.39	A
ATOM	1418	N	PRO	A	183	-11.899	-22.371	-25.856	1.00	21.32	A
ATOM	1419	CA	PRO	A	183	-10.802	-22.220	-25.296	1.00	22.60	A
ATOM	1420	CB	ILE	A	184	-12.748	-23.327	-25.517	1.00	21.08	A
ATOM	1421	CG	ILE	A	184	-12.345	-24.269	-24.494	1.00	23.29	A
ATOM	1422	O	ILE	A	184	-13.118	-24.019	-23.185	1.00	22.91	A
ATOM	1423	CG2	ILE	A	184	-12.720	-22.669	-23.621	1.00	23.87	A
ATOM	1424	CG1	ILE	A	184	-14.624	-24.034	-23.439	1.00	24.45	A
ATOM	1425	CD1	ILE	A	184	-15.454	-23.874	-22.154	1.00	28.40	A
ATOM	1426	C	ILE	A	184	-12.427	-25.733	-24.928	1.00	23.80	A
ATOM	1427	O	ILE	A	184	-12.332	-26.637	-24.103	1.00	24.50	A
ATOM	1428	N	GLY	A	185	-12.597	-25.964	-26.225	1.00	26.05	A
ATOM	1429	CA	GLY	A	185	-12.600	-27.329	-26.740	1.00	25.71	A
ATOM	1430	CB	GLY	A	185	-13.698	-28.288	-26.348	1.00	27.58	A
ATOM	1431	O	GLY	A	185	-13.512	-29.516	-26.410	1.00	27.68	A
ATOM	1432	N	GLN	A	186	-14.844	-27.738	-25.968	1.00	26.74	A
ATOM	1433	CA	GLN	A	186	-16.006	-28.518	-25.573	1.00	27.53	A
ATOM	1434	CB	GLN	A	186	-16.150	-28.518	-24.048	1.00	28.12	A
ATOM	1435	CG	GLN	A	186	-14.938	-29.039	-23.330	1.00	28.26	A
ATOM	1436	CD	GLN	A	186	-14.790	-28.436	-21.949	1.00	29.33	A
ATOM	1437	OE1	GLN	A	186	-15.532	-28.775	-21.025	1.00	28.19	A
ATOM	1438	NE2	GLN	A	186	-13.834	-27.525	-21.808	1.00	29.64	A
ATOM	1439	C	GLN	A	186	-17.217	-27.837	-26.192	1.00	27.94	A
ATOM	1440	O	GLN	A	186	-17.297	-26.613	-26.227	1.00	27.59	A
ATOM	1441	N	SER	A	187	-18.156	-28.632	-26.687	1.00	29.04	A
ATOM	1442	CA	SER	A	187	-19.368	-28.105	-27.290	1.00	28.26	A
ATOM	1443	CB	SER	A	187	-19.987	-29.173	-28.202	1.00	30.89	A
ATOM	1444	CG	SER	A	187	-21.163	-28.684	-28.826	1.00	35.18	A
ATOM	1445	O	SER	A	187	-20.294	-27.770	-26.120	1.00	27.81	A
ATOM	1446	N	SER	A	187	-20.650	-28.652	-25.339	1.00	28.41	A
ATOM	1447	CA	LEU	A	188	-20.681	-26.502	-26.000	1.00	25.54	A
ATOM	1448	CB	LEU	A	188	-21.504	-26.055	-24.875	1.00	23.98	A
ATOM	1449	CG	LEU	A	188	-20.785	-24.911	-24.136	1.00	23.58	A
ATOM	1450	CD1	LEU	A	188	-19.296	-25.012	-23.823	1.00	23.00	A
ATOM	1451	CD2	LEU	A	188	-18.653	-23.602	-23.655	1.00	22.33	A
ATOM	1452	C	LEU	A	188	-19.138	-25.849	-22.567	1.00	23.44	A
ATOM	1453	O	LEU	A	188	-22.883	-25.548	-25.235	1.00	24.43	A
ATOM	1454	N	LEU	A	188	-23.105	-25.040	-26.341	1.00	23.24	A
ATOM	1455	CA	PRO	A	189	-23.843	-25.694	-24.308	1.00	24.44	A
ATOM	1456	CB	PRO	A	189	-23.775	-26.479	-23.057	1.00	26.09	A
ATOM	1457	CG	PRO	A	189	-25.204	-25.207	-24.547	1.00	24.88	A
ATOM	1458	O	PRO	A	189	-26.014	-25.858	-23.420	1.00	26.37	A
ATOM	1459	C	PRO	A	189	-25.007	-25.986	-22.303	1.00	25.65	A
ATOM	1460	N	PRO	A	189	-25.111	-23.687	-24.375	1.00	25.47	A
ATOM	1461	CA	SER	A	190	-24.212	-23.195	-23.668	1.00	24.66	A
ATOM	1462	CB	SER	A	190	-26.019	-22.948	-25.005	1.00	25.63	A
ATOM	1463	CG	SER	A	190	-26.009	-21.492	-24.887	1.00	25.88	A
ATOM	1464	O	SER	A	190	-26.878	-20.866	-25.960	1.00	26.21	A
ATOM	1465	OG	SER	A	190	-26.413	-21.232	-27.230	1.00	31.10	A

Figure 1 (continued 15)

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ATOM	1466	C	SER	A	190	-26.546	-21.121	-23.537	1.00	25.83	A
ATOM	1467	O	SER	A	190	-27.690	-21.444	-23.194	1.00	26.64	A
ATOM	1468	N	HIS	A	191	-25.741	-20.414	-22.757	1.00	24.59	A
ATOM	1469	CA	HIS	A	191	-26.179	-20.046	-21.424	1.00	23.84	A
ATOM	1470	CB	HIS	A	191	-25.761	-21.123	-20.433	1.00	28.01	A
ATOM	1471	CG	HIS	A	191	-26.680	-21.250	-19.267	1.00	33.05	A
ATOM	1472	CD2	HIS	A	191	-26.528	-20.901	-17.966	1.00	33.83	A
ATOM	1473	ND1	HIS	A	191	-27.956	-21.759	-19.383	1.00	34.03	A
ATOM	1474	CE1	HIS	A	191	-28.552	-21.716	-18.202	1.00	34.58	A
ATOM	1475	NE2	HIS	A	191	-27.708	-21.200	-17.326	1.00	35.13	A
ATOM	1476	C	HIS	A	191	-25.529	-18.727	-21.035	1.00	21.91	A
ATOM	1477	O	HIS	A	191	-24.404	-18.450	-21.444	1.00	19.14	A
ATOM	1478	N	SER	A	192	-26.236	-17.937	-20.238	1.00	18.95	A
ATOM	1479	CA	SER	A	192	-25.741	-16.633	-19.821	1.00	19.59	A
ATOM	1480	CB	SER	A	192	-26.394	-15.574	-20.743	1.00	22.50	A
ATOM	1481	OG	SER	A	192	-26.222	-14.238	-20.342	1.00	27.62	A
ATOM	1482	C	SER	A	192	-26.135	-16.407	-18.360	1.00	19.05	A
ATOM	1483	O	SER	A	192	-27.304	-16.593	-18.004	1.00	21.16	A
ATOM	1484	N	VAL	A	193	-25.165	-16.043	-17.524	1.00	16.50	A
ATOM	1485	CA	VAL	A	193	-25.407	-15.734	-16.095	1.00	14.76	A
ATOM	1486	CB	VAL	A	193	-25.093	-16.937	-15.138	1.00	13.63	A
ATOM	1487	CG1	VAL	A	193	-25.999	-18.109	-15.494	1.00	17.20	A
ATOM	1488	CG2	VAL	A	193	-23.620	-17.348	-15.216	1.00	15.41	A
ATOM	1489	C	VAL	A	193	-24.538	-14.560	-15.664	1.00	14.41	A
ATOM	1490	O	VAL	A	193	-23.516	-14.254	-16.291	1.00	12.96	A
ATOM	1491	N	ILE	A	194	-24.968	-13.886	-14.607	1.00	12.61	A
ATOM	1492	CA	ILE	A	194	-24.252	-12.716	-14.085	1.00	11.47	A
ATOM	1493	CB	ILE	A	194	-25.213	-11.508	-13.867	1.00	12.39	A
ATOM	1494	CG2	ILE	A	194	-24.396	-10.299	-13.430	1.00	12.88	A
ATOM	1495	CG1	ILE	A	194	-25.983	-11.198	-15.146	1.00	14.24	A
ATOM	1496	CD1	ILE	A	194	-27.031	-10.095	-14.967	1.00	17.17	A
ATOM	1497	C	ILE	A	194	-23.660	-13.080	-12.736	1.00	13.07	A
ATOM	1498	O	ILE	A	194	-24.376	-13.466	-11.803	1.00	13.64	A
ATOM	1499	N	VAL	A	195	-22.336	-13.004	-12.632	1.00	12.90	A
ATOM	1500	CA	VAL	A	195	-21.654	-13.314	-11.385	1.00	14.01	A
ATOM	1501	CB	VAL	A	195	-20.301	-14.008	-11.696	1.00	15.92	A
ATOM	1502	CG1	VAL	A	195	-19.560	-14.344	-10.413	1.00	14.56	A
ATOM	1503	CG2	VAL	A	195	-20.545	-15.287	-12.497	1.00	13.57	A
ATOM	1504	C	VAL	A	195	-21.424	-11.989	-10.641	1.00	13.97	A
ATOM	1505	O	VAL	A	195	-20.949	-11.041	-11.214	1.00	14.63	A
ATOM	1506	N	PRO	A	196	-21.783	-11.915	-9.351	1.00	15.51	A
ATOM	1507	CD	PRO	A	196	-22.324	-12.986	-8.492	1.00	16.27	A
ATOM	1508	CA	PRO	A	196	-21.573	-10.657	-8.622	1.00	16.07	A
ATOM	1509	CB	PRO	A	196	-22.178	-10.929	-7.241	1.00	17.85	A
ATOM	1510	CG	PRO	A	196	-22.132	-12.418	-7.098	1.00	18.14	A
ATOM	1511	C	PRO	A	196	-20.114	-10.220	-8.553	1.00	16.89	A
ATOM	1512	O	PRO	A	196	-19.202	-11.051	-8.543	1.00	15.71	A
ATOM	1513	N	ARG	A	197	-19.868	-8.916	-8.473	1.00	17.07	A
ATOM	1514	CA	ARG	A	197	-18.470	-8.494	-8.456	1.00	19.18	A
ATOM	1515	CB	ARG	A	197	-18.351	-6.965	-8.477	1.00	23.00	A
ATOM	1516	CG	ARG	A	197	-19.035	-6.236	-7.375	1.00	26.04	A
ATOM	1517	CD	ARG	A	197	-18.680	-4.725	-7.481	1.00	28.79	A
ATOM	1518	NE	ARG	A	197	-17.228	-4.495	-7.441	1.00	32.92	A
ATOM	1519	CZ	ARG	A	197	-16.496	-4.048	-8.463	1.00	34.73	A
ATOM	1520	NH1	ARG	A	197	-17.059	-3.761	-9.628	1.00	36.57	A
ATOM	1521	NH2	ARG	A	197	-15.185	-3.905	-8.329	1.00	37.08	A
ATOM	1522	C	ARG	A	197	-17.590	-9.107	-7.376	1.00	18.61	A
ATOM	1523	O	ARG	A	197	-16.447	-9.437	-7.645	1.00	19.10	A
ATOM	1524	N	LYS	A	198	-18.106	-9.310	-6.165	1.00	19.11	A
ATOM	1525	CA	LYS	A	198	-17.295	-9.924	-5.130	1.00	21.70	A
ATOM	1526	CB	LYS	A	198	-18.032	-9.861	-3.790	1.00	24.75	A
ATOM	1527	CG	LYS	A	198	-17.243	-10.408	-2.616	1.00	30.79	A
ATOM	1528	CD	LYS	A	198	-17.904	-9.948	-1.300	1.00	32.84	A
ATOM	1529	CE	LYS	A	198	-17.265	-10.606	-0.086	1.00	35.71	A
ATOM	1530	NZ	LYS	A	198	-17.913	-10.169	1.206	1.00	35.61	A
ATOM	1531	C	LYS	A	198	-16.943	-11.377	-5.492	1.00	20.89	A
ATOM	1532	O	LYS	A	198	-15.864	-11.885	-5.152	1.00	21.60	A
ATOM	1533	N	GLY	A	199	-17.844	-12.052	-6.205	1.00	19.66	A
ATOM	1534	CA	GLY	A	199	-17.583	-13.421	-6.613	1.00	18.99	A
ATOM	1535	C	GLY	A	199	-16.488	-13.483	-7.678	1.00	17.60	A
ATOM	1536	O	GLY	A	199	-15.678	-14.406	-7.751	1.00	18.00	A
ATOM	1537	N	VAL	A	200	-16.492	-12.486	-8.553	1.00	18.22	A
ATOM	1538	CA	VAL	A	200	-15.498	-12.422	-9.610	1.00	16.49	A
ATOM	1539	CB	VAL	A	200	-15.780	-11.199	-10.534	1.00	15.63	A
ATOM	1540	CG1	VAL	A	200	-14.604	-11.013	-11.522	1.00	16.76	A
ATOM	1541	CG2	VAL	A	200	-17.104	-11.417	-11.287	1.00	17.52	A
ATOM	1542	C	VAL	A	200	-14.097	-12.289	-8.978	1.00	18.83	A
ATOM	1543	O	VAL	A	200	-13.138	-12.928	-9.425	1.00	19.59	A
ATOM	1544	N	ILE	A	201	-14.002	-11.465	-7.937	1.00	21.69	A
ATOM	1545	CA	ILE	A	201	-12.735	-11.240	-7.220	1.00	24.32	A
ATOM	1546	CB	ILE	A	201	-12.897	-10.278	-6.026	1.00	26.86	A
ATOM	1547	CG2	ILE	A	201	-11.547	-10.101	-5.327	1.00	28.23	A
ATOM	1548	CG1	ILE	A	201	-13.504	-8.954	-6.471	1.00	28.44	A
ATOM	1549	CD1	ILE	A	201	-13.047	-8.463	-7.799	1.00	29.79	A
ATOM	1550	C	ILE	A	201	-12.227	-12.531	-6.619	1.00	24.50	A
ATOM	1551	O	ILE	A	201	-11.042	-12.872	-6.721	1.00	24.04	A
ATOM	1552	N	GLU	A	202	-13.141	-13.234	-5.971	1.00	26.55	A
ATOM	1553	CA	GLU	A	202	-12.854	-14.491	-5.319	1.00	29.06	A
ATOM	1554	CB	GLU	A	202	-14.113	-14.972	-4.574	1.00	32.98	A
ATOM	1555	CG	GLU	A	202	-13.831	-15.705	-3.291	1.00	36.13	A
ATOM	1556	CD	GLU	A	202	-12.688	-15.076	-2.521	1.00	38.29	A
ATOM	1557	OE1	GLU	A	202	-12.804	-13.893	-2.097	1.00	38.50	A
ATOM	1558	OE2	GLU	A	202	-11.665	-15.777	-2.356	1.00	39.57	A
ATOM	1559	C	GLU	A	202	-12.405	-15.522	-6.346	1.00	29.59	A
ATOM	1560	O	GLU	A	202	-11.447	-15.263	-6.117	1.00	29.66	A
ATOM	1561	N	LEU	A	203	-13.080	-15.573	-7.490	1.00	28.27	A
ATOM	1562	CA	LEU	A	203	-12.706	-16.519	-8.529	1.00	28.89	A
ATOM	1563	CB	LEU	A	203	-13.595	-16.352	-9.761	1.00	31.21	A
ATOM	1564	CG	LEU	A	203	-14.700	-17.368	-10.014	1.00	31.78	A
ATOM	1565	CD1	LEU	A	203	-15.388	-17.044	-11.313	1.00	30.83	A

Figure 1 (continued 16)

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ATOM	1566	CD2	LEU	A	203	-14.090	-18.768	-10.061	1.00	32.03	A
ATOM	1567	C	LEU	A	203	-11.260	-16.256	-8.929	1.00	29.61	A
ATOM	1568	O	LEU	A	203	-10.459	-17.171	-9.072	1.00	27.41	A
ATOM	1569	N	MET	A	204	-10.951	-14.984	-9.134	1.00	28.89	A
ATOM	1570	CA	MET	A	204	-9.615	-14.578	-9.514	1.00	31.07	A
ATOM	1571	CB	MET	A	204	-9.589	-13.048	-9.635	1.00	32.20	A
ATOM	1572	CG	MET	A	204	-8.538	-12.491	-10.565	1.00	36.14	A
ATOM	1573	SD	MET	A	204	-8.637	-13.238	-12.199	1.00	37.25	A
ATOM	1574	CE	MET	A	204	-7.159	-14.209	-12.153	1.00	38.24	A
ATOM	1575	C	MET	A	204	-8.599	-15.060	-8.463	1.00	32.05	A
ATOM	1576	O	MET	A	204	-7.545	-15.592	-8.813	1.00	31.41	A
ATOM	1577	N	ARG	A	205	-8.936	-14.905	-7.182	1.00	33.59	A
ATOM	1578	CA	ARG	A	205	-8.040	-15.287	-6.071	1.00	36.58	A
ATOM	1579	CB	ARG	A	205	-8.659	-14.940	-4.707	1.00	38.43	A
ATOM	1580	CG	ARG	A	205	-9.093	-13.505	-4.521	1.00	42.16	A
ATOM	1581	CD	ARG	A	205	-7.928	-12.549	-4.307	1.00	45.61	A
ATOM	1582	NE	ARG	A	205	-8.409	-11.165	-4.316	1.00	47.97	A
ATOM	1583	CZ	ARG	A	205	-7.674	-10.093	-4.029	1.00	48.71	A
ATOM	1584	NH1	ARG	A	205	-6.392	-10.219	-3.694	1.00	49.29	A
ATOM	1585	NH2	ARG	A	205	-8.227	-8.886	-4.092	1.00	37.14	A
ATOM	1586	C	ARG	A	205	-7.643	-16.752	-6.002	1.00	37.07	A
ATOM	1587	O	ARG	A	205	-6.571	-17.088	-5.492	1.00	37.50	A
ATOM	1588	N	MET	A	206	-8.496	-17.641	-6.482	1.00	39.03	A
ATOM	1589	CA	MET	A	206	-8.162	-19.049	-6.380	1.00	39.34	A
ATOM	1590	CB	MET	A	206	-9.435	-19.869	-6.144	1.00	39.33	A
ATOM	1591	CG	MET	A	206	-10.340	-19.984	-7.341	1.00	39.83	A
ATOM	1592	SD	MET	A	206	-11.995	-20.514	-6.828	1.00	37.83	A
ATOM	1593	CE	MET	A	206	-11.592	-22.096	-5.995	1.00	40.42	A
ATOM	1594	C	MET	A	206	-7.403	-19.572	-7.587	1.00	39.42	A
ATOM	1595	O	MET	A	206	-7.071	-20.759	-7.657	1.00	41.79	A
ATOM	1596	N	LEU	A	207	-7.117	-18.686	-8.534	1.00	45.36	A
ATOM	1597	CA	LEU	A	207	-6.403	-19.081	-9.744	1.00	45.10	A
ATOM	1598	CB	LEU	A	207	-6.972	-18.329	-10.755	1.00	46.04	A
ATOM	1599	CG	LEU	A	207	-8.187	-18.866	-11.721	1.00	45.64	A
ATOM	1600	CD1	LEU	A	207	-9.219	-19.475	-10.799	1.00	46.42	A
ATOM	1601	CD2	LEU	A	207	-8.791	-17.719	-12.517	1.00	47.44	A
ATOM	1602	C	LEU	A	207	-4.903	-18.814	-9.629	1.00	48.80	A
ATOM	1603	O	LEU	A	207	-4.487	-17.670	-9.432	1.00	49.36	A
ATOM	1604	N	ASP	A	208	-4.103	-19.869	-9.761	1.00	51.16	A
ATOM	1605	CA	ASP	A	208	-2.648	-19.759	-9.681	1.00	52.20	A
ATOM	1606	CB	ASP	A	208	-2.126	-20.579	-8.504	1.00	54.01	A
ATOM	1607	CG	ASP	A	208	-2.697	-20.119	-7.180	1.00	54.78	A
ATOM	1608	OD1	ASP	A	208	-2.638	-18.896	-6.906	1.00	53.95	A
ATOM	1609	OD2	ASP	A	208	-3.198	-20.978	-6.412	1.00	51.89	A
ATOM	1610	C	ASP	A	208	-1.954	-20.216	-10.967	1.00	52.13	A
ATOM	1611	O	ASP	A	208	-0.786	-20.611	-10.950	1.00	52.31	A
ATOM	1612	N	GLY	A	209	-2.689	-20.168	-12.076	1.00	52.06	A
ATOM	1613	CA	GLY	A	209	-2.144	-20.552	-13.366	1.00	52.17	A
ATOM	1614	C	GLY	A	209	-1.567	-21.948	-13.502	1.00	52.89	A
ATOM	1615	O	GLY	A	209	-0.961	-22.254	-14.533	1.00	51.34	A
ATOM	1616	N	GLY	A	210	-1.737	-22.795	-12.488	1.00	50.65	A
ATOM	1617	CA	GLY	A	210	-1.215	-24.152	-12.566	1.00	49.99	A
ATOM	1618	C	GLY	A	210	-1.779	-24.891	-13.769	1.00	49.83	A
ATOM	1619	O	GLY	A	210	-2.751	-24.435	-14.367	1.00	49.29	A
ATOM	1620	N	ASP	A	211	-1.180	-26.023	-14.135	1.00	48.42	A
ATOM	1621	CA	ASP	A	211	-1.656	-26.803	-15.283	1.00	49.93	A
ATOM	1622	CB	ASP	A	211	-0.602	-27.833	-15.701	1.00	51.04	A
ATOM	1623	CG	ASP	A	211	0.655	-27.184	-16.261	1.00	52.21	A
ATOM	1624	OD1	ASP	A	211	0.568	-26.549	-17.334	1.00	53.08	A
ATOM	1625	OD2	ASP	A	211	1.725	-27.303	-15.627	1.00	47.33	A
ATOM	1626	C	ASP	A	211	-2.953	-27.508	-14.910	1.00	47.11	A
ATOM	1627	O	ASN	A	212	-3.642	-28.077	-15.759	1.00	45.10	A
ATOM	1628	CA	ASN	A	212	-3.247	-27.442	-13.616	1.00	43.75	A
ATOM	1629	N	ASN	A	212	-4.425	-28.013	-12.974	1.00	44.05	A
ATOM	1630	CB	ASN	A	212	-4.245	-27.801	-11.463	1.00	45.06	A
ATOM	1631	CG	ASN	A	212	-5.009	-28.795	-10.619	1.00	44.49	A
ATOM	1632	OD1	ASN	A	212	-4.957	-28.731	-9.387	1.00	45.44	A
ATOM	1633	ND2	ASN	A	212	-5.715	-29.722	-11.263	1.00	41.13	A
ATOM	1634	C	ASN	A	212	-5.653	-27.237	-13.497	1.00	42.29	A
ATOM	1635	O	ASN	A	212	-5.779	-26.045	-13.252	1.00	38.67	A
ATOM	1636	N	PRO	A	213	-6.573	-27.899	-14.221	1.00	38.16	A
ATOM	1637	CD	PRO	A	213	-6.625	-29.292	-14.698	1.00	35.46	A
ATOM	1638	CA	PRO	A	213	-7.731	-27.143	-14.716	1.00	36.69	A
ATOM	1639	CB	PRO	A	213	-8.264	-28.026	-15.829	1.00	38.80	A
ATOM	1640	CG	PRO	A	213	-8.037	-29.389	-15.267	1.00	32.37	A
ATOM	1641	C	PRO	A	213	-8.806	-26.834	-13.686	1.00	32.62	A
ATOM	1642	O	PRO	A	213	-8.897	-27.468	-12.635	1.00	29.01	A
ATOM	1643	N	LEU	A	214	-9.622	-25.840	-14.013	1.00	26.42	A
ATOM	1644	CA	LEU	A	214	-10.734	-25.415	-13.172	1.00	27.73	A
ATOM	1645	CB	LEU	A	214	-10.934	-23.896	-13.338	1.00	29.04	A
ATOM	1646	CG	LEU	A	214	-12.055	-23.149	-12.622	1.00	31.24	A
ATOM	1647	CD1	LEU	A	214	-11.718	-23.086	-11.170	1.00	29.62	A
ATOM	1648	CD2	LEU	A	214	-12.194	-21.719	-13.164	1.00	24.15	A
ATOM	1649	C	LEU	A	214	-11.979	-26.163	-13.663	1.00	23.32	A
ATOM	1650	O	LEU	A	214	-12.179	-26.296	-14.867	1.00	20.02	A
ATOM	1651	N	ARG	A	215	-12.803	-26.670	-12.751	1.00	20.46	A
ATOM	1652	CA	ARG	A	215	-14.025	-27.355	-13.139	1.00	25.18	A
ATOM	1653	CB	ARG	A	215	-14.132	-28.715	-12.415	1.00	31.55	A
ATOM	1654	CG	ARG	A	215	-12.876	-29.577	-12.626	1.00	37.20	A
ATOM	1655	CD	ARG	A	215	-13.031	-31.025	-12.142	1.00	42.35	A
ATOM	1656	NE	ARG	A	215	-13.414	-31.946	-13.221	1.00	44.98	A
ATOM	1657	CZ	ARG	A	215	-14.626	-32.003	-13.779	1.00	46.39	A
ATOM	1658	NH1	ARG	A	215	-15.597	-31.192	-13.360	1.00	44.99	A
ATOM	1659	NH2	ARG	A	215	-14.871	-32.862	-14.771	1.00	18.21	A
ATOM	1660	C	ARG	A	215	-15.158	-26.422	-12.724	1.00	18.66	A
ATOM	1661	O	ARG	A	215	-15.280	-26.064	-11.564	1.00	15.42	A
ATOM	1662	N	VAL	A	216	-15.978	-26.026	-13.682	1.00	15.50	A
ATOM	1663	CA	VAL	A	216	-17.061	-25.082	-13.410	1.00	14.33	A
ATOM	1664	CB	VAL	A	216	-16.988	-23.890	-14.404	1.00	16.88	A
ATOM	1665	CG1	VAL	A	216	-18.154	-22.945	-14.149	1.00		

Figure 1 (continued 17)

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ATOM	1666	CG2	VAL	A	216	-15.661	-23.199	-14.269	1.00	16.10	A
ATOM	1667	C	VAL	A	216	-18.420	-25.727	-13.568	1.00	15.31	A
ATOM	1668	O	VAL	A	216	-18.641	-26.525	-14.488	1.00	18.21	A
ATOM	1669	N	GLN	A	217	-19.347	-25.373	-12.680	1.00	15.12	A
ATOM	1670	CA	GLN	A	217	-20.696	-25.879	-12.745	1.00	16.55	A
ATOM	1671	CB	GLN	A	217	-21.001	-26.859	-11.607	1.00	17.03	A
ATOM	1672	CG	GLN	A	217	-20.322	-28.182	-11.686	1.00	17.24	A
ATOM	1673	CD	GLN	A	217	-20.607	-29.052	-10.445	1.00	19.83	A
ATOM	1674	OE1	GLN	A	217	-20.179	-28.723	-9.334	1.00	24.33	A
ATOM	1675	NE2	GLN	A	217	-21.341	-30.150	-10.636	1.00	22.05	A
ATOM	1676	O	GLN	A	217	-21.590	-24.655	-12.596	1.00	16.13	A
ATOM	1677	N	ILE	A	218	-21.412	-23.872	-11.675	1.00	16.81	A
ATOM	1678	CA	ILE	A	218	-22.543	-24.485	-13.510	1.00	16.16	A
ATOM	1679	CB	ILE	A	218	-23.457	-23.338	-13.436	1.00	17.93	A
ATOM	1680	CG	ILE	A	218	-23.312	-22.443	-14.721	1.00	17.67	A
ATOM	1681	CG2	ILE	A	218	-24.342	-21.285	-14.709	1.00	19.90	A
ATOM	1682	CG1	ILE	A	218	-21.885	-21.891	-14.797	1.00	18.86	A
ATOM	1683	CD1	ILE	A	218	-21.559	-21.069	-16.069	1.00	20.21	A
ATOM	1684	O	ILE	A	218	-24.895	-23.824	-13.317	1.00	16.21	A
ATOM	1685	N	ILE	A	218	-25.327	-24.690	-14.080	1.00	17.78	A
ATOM	1686	CA	GLY	A	219	-25.622	-23.261	-12.357	1.00	17.39	A
ATOM	1687	CB	GLY	A	219	-27.028	-23.573	-12.144	1.00	17.69	A
ATOM	1688	CG	GLY	A	219	-27.886	-22.361	-12.487	1.00	19.32	A
ATOM	1689	CD	GLY	A	219	-27.381	-21.370	-12.982	1.00	20.27	A
ATOM	1690	O	SER	A	220	-29.188	-22.425	-12.243	1.00	20.22	A
ATOM	1691	CA	SER	A	220	-30.033	-21.285	-12.570	1.00	21.44	A
ATOM	1692	CB	SER	A	220	-31.498	-21.655	-12.408	1.00	22.40	A
ATOM	1693	CG	SER	A	220	-31.780	-22.064	-11.071	1.00	25.42	A
ATOM	1694	CD	SER	A	220	-29.741	-20.079	-11.690	1.00	21.28	A
ATOM	1695	O	SER	A	220	-29.925	-18.935	-12.113	1.00	20.79	A
ATOM	1696	N	ASN	A	221	-29.283	-20.337	-10.470	1.00	19.85	A
ATOM	1697	CA	ASN	A	221	-29.033	-19.257	-9.523	1.00	20.14	A
ATOM	1698	CB	ASN	A	221	-30.174	-19.212	-8.498	1.00	23.10	A
ATOM	1699	CG	ASN	A	221	-31.536	-18.962	-9.162	1.00	26.82	A
ATOM	1700	OD1	ASN	A	221	-32.207	-19.897	-9.622	1.00	31.73	A
ATOM	1701	ND2	ASN	A	221	-31.927	-17.700	-9.245	1.00	27.82	A
ATOM	1702	C	ASN	A	221	-27.704	-19.312	-7.798	1.00	17.29	A
ATOM	1703	O	ASN	A	221	-27.487	-18.567	-7.845	1.00	16.83	A
ATOM	1704	N	ASN	A	222	-26.814	-20.188	-9.249	1.00	16.78	A
ATOM	1705	CA	ASN	A	222	-25.523	-20.298	-8.582	1.00	15.72	A
ATOM	1706	CB	ASN	A	222	-25.543	-21.424	-7.526	1.00	18.61	A
ATOM	1707	CG	ASN	A	222	-26.571	-21.210	-6.432	1.00	20.68	A
ATOM	1708	OD1	ASN	A	222	-27.756	-21.491	-6.615	1.00	22.08	A
ATOM	1709	ND2	ASN	A	222	-26.125	-20.705	-5.297	1.00	23.78	A
ATOM	1710	C	ASN	A	222	-24.439	-20.686	-9.564	1.00	13.83	A
ATOM	1711	O	ASN	A	222	-24.736	-21.188	-10.637	1.00	14.52	A
ATOM	1712	N	ILE	A	223	-23.170	-30.449	-9.191	1.00	12.97	A
ATOM	1713	CA	ILE	A	223	-22.034	-20.910	-10.008	1.00	13.44	A
ATOM	1714	CB	ILE	A	223	-21.357	-19.742	-10.831	1.00	12.76	A
ATOM	1715	CG2	ILE	A	223	-20.893	-18.636	-9.884	1.00	13.49	A
ATOM	1716	CG1	ILE	A	223	-20.166	-20.277	-11.648	1.00	13.07	A
ATOM	1717	CD1	ILE	A	223	-19.880	-19.360	-12.824	1.00	15.33	A
ATOM	1718	O	ILE	A	223	-21.027	-21.498	-8.989	1.00	13.40	A
ATOM	1719	N	ARG	A	224	-20.860	-20.994	-7.866	1.00	13.37	A
ATOM	1720	CA	ARG	A	224	-20.173	-22.578	-9.388	1.00	12.68	A
ATOM	1721	CB	ARG	A	224	-19.398	-23.229	-8.544	1.00	13.73	A
ATOM	1722	CG	ARG	A	224	-19.948	-24.578	-8.058	1.00	16.50	A
ATOM	1723	CD	ARG	A	224	-18.928	-25.397	-7.280	1.00	18.24	A
ATOM	1724	NE	ARG	A	224	-19.612	-26.522	-6.521	1.00	21.35	A
ATOM	1725	CZ	ARG	A	224	-20.401	-25.966	-5.432	1.00	23.07	A
ATOM	1726	NH1	ARG	A	224	-21.253	-26.655	-4.680	1.00	25.49	A
ATOM	1727	NH2	ARG	A	224	-21.440	-27.954	-4.897	1.00	27.26	A
ATOM	1728	O	ARG	A	224	-21.935	-26.039	-3.721	1.00	27.55	A
ATOM	1729	C	ARG	A	224	-18.152	-23.471	-9.370	1.00	13.92	A
ATOM	1730	N	ALA	A	225	-18.217	-23.780	-10.567	1.00	13.44	A
ATOM	1731	CA	ALA	A	225	-17.014	-23.302	-8.723	1.00	13.45	A
ATOM	1732	CB	ALA	A	225	-15.738	-23.582	-9.362	1.00	15.31	A
ATOM	1733	CG	ALA	A	225	-15.027	-22.310	-9.670	1.00	16.60	A
ATOM	1734	CD	ALA	A	225	-14.892	-24.435	-8.419	1.00	16.41	A
ATOM	1735	O	ALA	A	225	-14.763	-24.128	-7.236	1.00	15.00	A
ATOM	1736	N	HIS	A	226	-14.310	-25.501	-8.961	1.00	17.50	A
ATOM	1737	CA	HIS	A	226	-13.467	-26.417	-8.187	1.00	19.53	A
ATOM	1738	CB	HIS	A	226	-13.896	-27.882	-8.433	1.00	23.40	A
ATOM	1739	CG	HIS	A	226	-15.351	-28.163	-8.216	1.00	24.26	A
ATOM	1740	CD2	HIS	A	226	-16.444	-27.890	-8.972	1.00	26.04	A
ATOM	1741	ND1	HIS	A	226	-15.813	-28.853	-7.111	1.00	26.55	A
ATOM	1742	CE1	HIS	A	226	-17.123	-28.994	-7.194	1.00	26.31	A
ATOM	1743	NE2	HIS	A	226	-17.532	-28.420	-8.314	1.00	27.11	A
ATOM	1744	C	HIS	A	226	-12.027	-26.291	-8.703	1.00	22.32	A
ATOM	1745	O	HIS	A	226	-11.794	-26.492	-9.899	1.00	21.45	A
ATOM	1746	N	VAL	A	227	-11.077	-25.951	-7.832	1.00	22.02	A
ATOM	1747	CA	VAL	A	227	-9.660	-25.869	-8.218	1.00	26.25	A
ATOM	1748	CB	VAL	A	227	-9.119	-24.414	-8.243	1.00	28.90	A
ATOM	1749	CG1	VAL	A	227	-7.857	-24.334	-9.076	1.00	30.53	A
ATOM	1750	CG2	VAL	A	227	-10.153	-23.489	-8.788	1.00	31.33	A
ATOM	1751	C	VAL	A	227	-8.913	-26.600	-7.121	1.00	26.06	A
ATOM	1752	O	VAL	A	227	-8.965	-26.192	-5.963	1.00	25.67	A
ATOM	1753	N	GLY	A	228	-8.197	-27.651	-7.480	1.00	25.91	A
ATOM	1754	CA	GLY	A	228	-7.468	-28.410	-6.478	1.00	24.98	A
ATOM	1755	C	GLY	A	228	-8.417	-28.855	-5.381	1.00	24.00	A
ATOM	1756	O	GLY	A	228	-9.469	-29.398	-5.671	1.00	24.36	A
ATOM	1757	N	ASP	A	229	-8.079	-28.595	-4.126	1.00	22.64	A
ATOM	1758	CA	ASP	A	229	-8.978	-29.011	-3.059	1.00	22.40	A
ATOM	1759	CB	ASP	A	229	-8.214	-29.766	-1.989	1.00	24.16	A
ATOM	1760	CG	ASP	A	229	-7.531	-31.019	-2.540	1.00	26.13	A
ATOM	1761	OD1	ASP	A	229	-8.128	-31.718	-3.399	1.00	27.09	A
ATOM	1762	OD2	ASP	A	229	-6.395	-31.293	-2.106	1.00	28.22	A
ATOM	1763	C	ASP	A	229	-9.760	-27.837	-2.470	1.00	21.77	A
ATOM	1764	O	ASP	A	229	-10.066	-27.791	-1.262	1.00	23.00	A
ATOM	1765	N	PHE	A	230	-10.049	-26.873	-3.334	1.00	20.12	A

Figure 1 (continued 18)

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ATOM	1766	CA	PHE	A	230	-10.841	-25.701	-2.949	1.00	20.28	A
ATOM	1767	CB	PHE	A	230	-10.082	-24.407	-3.238	1.00	20.97	A
ATOM	1768	CG	PHE	A	230	-8.878	-24.208	-2.391	1.00	20.97	A
ATOM	1769	CD1	PHE	A	230	-8.991	-23.676	-1.118	1.00	25.22	A
ATOM	1770	CD2	PHE	A	230	-7.621	-24.553	-2.865	1.00	26.34	A
ATOM	1771	CE1	PHE	A	230	-7.854	-23.486	-0.322	1.00	27.57	A
ATOM	1772	CE2	PHE	A	230	-6.474	-24.365	-2.071	1.00	26.07	A
ATOM	1773	CZ	PHE	A	230	-6.607	-23.828	-0.800	1.00	28.73	A
ATOM	1774	C	PHE	A	230	-12.113	-25.691	-3.786	1.00	25.38	A
ATOM	1775	O	PHE	A	230	-12.101	-26.051	-4.975	1.00	19.64	A
ATOM	1776	N	ILE	A	231	-13.221	-26.007	-3.156	1.00	18.35	A
ATOM	1777	CA	ILE	A	231	-14.492	-25.232	-3.873	1.00	16.55	A
ATOM	1778	CB	ILE	A	231	-15.467	-26.329	-3.471	1.00	16.98	A
ATOM	1779	CG2	ILE	A	231	-16.784	-26.149	-4.274	1.00	16.59	A
ATOM	1780	CG1	ILE	A	231	-14.856	-27.717	-3.733	1.00	16.05	A
ATOM	1781	CD1	ILE	A	231	-15.848	-28.868	-3.521	1.00	18.23	A
ATOM	1782	C	ILE	A	231	-15.136	-23.900	-3.555	1.00	21.86	A
ATOM	1783	O	ILE	A	231	-15.429	-23.581	-4.379	1.00	17.85	A
ATOM	1784	N	PHE	A	232	-15.326	-23.109	-4.609	1.00	18.50	A
ATOM	1785	CA	PHE	A	232	-15.943	-21.804	-5.281	1.00	15.87	A
ATOM	1786	CB	PHE	A	232	-15.150	-20.771	-4.487	1.00	15.49	A
ATOM	1787	CG	PHE	A	232	-15.792	-19.429	-5.269	1.00	15.94	A
ATOM	1788	CD1	PHE	A	232	-15.921	-18.748	-4.066	1.00	18.31	A
ATOM	1789	CD2	PHE	A	232	-16.283	-18.871	-6.431	1.00	20.92	A
ATOM	1790	CE1	PHE	A	232	-16.539	-17.502	-4.018	1.00	20.41	A
ATOM	1791	CE2	PHE	A	232	-16.915	-17.502	-6.399	1.00	21.57	A
ATOM	1792	CZ	PHE	A	232	-17.032	-16.929	-5.200	1.00	19.94	A
ATOM	1793	O	PHE	A	232	-17.349	-21.836	-5.060	1.00	21.00	A
ATOM	1794	N	THR	A	233	-17.556	-22.351	-6.142	1.00	14.79	A
ATOM	1795	CA	THR	A	233	-18.317	-21.261	-4.337	1.00	14.73	A
ATOM	1796	CB	THR	A	233	-19.683	-21.214	-4.858	1.00	13.80	A
ATOM	1797	OG1	THR	A	233	-20.616	-22.226	-4.151	1.00	14.57	A
ATOM	1798	CG2	THR	A	233	-20.009	-23.517	-4.157	1.00	16.94	A
ATOM	1799	C	THR	A	233	-21.972	-22.310	-4.883	1.00	17.68	A
ATOM	1800	O	THR	A	233	-20.236	-19.822	-4.603	1.00	17.95	A
ATOM	1801	N	SER	A	234	-20.018	-19.237	-3.544	1.00	14.93	A
ATOM	1802	CA	SER	A	234	-20.927	-19.274	-5.590	1.00	16.82	A
ATOM	1803	CB	SER	A	234	-21.543	-17.968	-5.406	1.00	14.49	A
ATOM	1804	OG	SER	A	234	-20.743	-16.883	-6.136	1.00	13.46	A
ATOM	1805	C	SER	A	234	-21.424	-15.612	-6.057	1.00	13.74	A
ATOM	1806	O	SER	A	234	-22.952	-17.945	-5.976	1.00	15.56	A
ATOM	1807	N	LYS	A	235	-23.272	-18.673	-6.914	1.00	13.72	A
ATOM	1808	CA	LYS	A	235	-23.796	-17.096	-5.384	1.00	14.31	A
ATOM	1809	CB	LYS	A	235	-25.140	-16.882	-5.941	1.00	14.72	A
ATOM	1810	CG	LYS	A	235	-26.017	-16.089	-4.965	1.00	15.52	A
ATOM	1811	CD	LYS	A	235	-26.346	-16.843	-3.692	1.00	18.32	A
ATOM	1812	CE	LYS	A	235	-27.446	-16.147	-2.881	1.00	22.03	A
ATOM	1813	CZ	LYS	A	235	-28.805	-16.273	-3.561	1.00	26.96	A
ATOM	1814	N	LYS	A	235	-29.279	-17.699	-3.762	1.00	31.30	A
ATOM	1815	CA	LYS	A	235	-24.904	-16.023	-7.181	1.00	34.33	A
ATOM	1816	CB	LEU	A	236	-23.843	-15.357	-7.310	1.00	13.85	A
ATOM	1817	CG	LEU	A	236	-25.865	-16.060	-8.109	1.00	14.11	A
ATOM	1818	CD1	LEU	A	236	-25.790	-15.236	-9.322	1.00	14.19	A
ATOM	1819	CD2	LEU	A	236	-26.307	-16.007	-10.538	1.00	14.29	A
ATOM	1820	C	LEU	A	236	-25.517	-17.278	-10.914	1.00	13.43	A
ATOM	1821	O	LEU	A	236	-26.211	-18.059	-12.011	1.00	15.03	A
ATOM	1822	N	LEU	A	236	-24.085	-16.907	-11.375	1.00	13.57	A
ATOM	1823	CA	VAL	A	237	-26.661	-14.004	-9.095	1.00	15.56	A
ATOM	1824	CB	VAL	A	237	-27.429	-13.931	-8.119	1.00	18.35	A
ATOM	1825	CG	VAL	A	237	-26.555	-13.052	-9.998	1.00	14.01	A
ATOM	1826	CD1	VAL	A	237	-27.324	-11.803	-9.903	1.00	17.40	A
ATOM	1827	CD2	VAL	A	237	-26.462	-10.592	-10.324	1.00	16.42	A
ATOM	1828	C	VAL	A	237	-27.275	-9.292	-10.179	1.00	18.55	A
ATOM	1829	O	VAL	A	237	-25.205	-10.504	-9.471	1.00	17.94	A
ATOM	1830	N	VAL	A	237	-28.516	-11.863	-10.844	1.00	19.10	A
ATOM	1831	CA	ASP	A	238	-28.394	-12.262	-12.003	1.00	19.48	A
ATOM	1832	CB	ASP	A	238	-29.683	-11.441	-10.368	1.00	23.53	A
ATOM	1833	CG	ASP	A	238	-30.842	-11.424	-11.253	1.00	27.58	A
ATOM	1834	CD	ASP	A	238	-32.129	-11.384	-10.441	1.00	31.74	A
ATOM	1835	CE	ASP	A	238	-33.093	-12.485	-10.849	1.00	36.33	A
ATOM	1836	CZ	ASP	A	238	-33.506	-12.522	-12.038	1.00	38.03	A
ATOM	1837	N	ASP	A	238	-33.429	-13.318	-9.979	1.00	39.43	A
ATOM	1838	CA	ASP	A	238	-30.788	-10.205	-12.193	1.00	27.85	A
ATOM	1839	CB	GLY	A	239	-30.073	-9.224	-11.951	1.00	27.68	A
ATOM	1840	CG	GLY	A	239	-31.516	-10.272	-13.288	1.00	27.65	A
ATOM	1841	CD	GLY	A	239	-31.524	-9.143	-14.185	1.00	27.62	A
ATOM	1842	CE	GLY	A	239	-31.152	-9.550	-15.580	1.00	28.08	A
ATOM	1843	CZ	GLY	A	239	-30.584	-10.616	-15.790	1.00	28.81	A
ATOM	1844	N	ARG	A	240	-31.491	-8.683	-16.521	1.00	29.63	A
ATOM	1845	CA	ARG	A	240	-31.208	-8.878	-17.932	1.00	30.14	A
ATOM	1846	CB	ARG	A	240	-32.392	-8.389	-18.771	1.00	33.69	A
ATOM	1847	CG	ARG	A	240	-32.239	-8.574	-20.279	1.00	38.96	A
ATOM	1848	CD	ARG	A	240	-32.122	-10.052	-20.651	1.00	43.41	A
ATOM	1849	CE	ARG	A	240	-32.302	-10.267	-22.087	1.00	46.82	A
ATOM	1850	CZ	ARG	A	240	-32.389	-11.460	-22.669	1.00	48.33	A
ATOM	1851	NH1	ARG	A	240	-32.313	-12.570	-21.944	1.00	49.90	A
ATOM	1852	NH2	ARG	A	240	-32.553	-11.543	-23.985	1.00	49.72	A
ATOM	1853	C	ARG	A	240	-29.980	-8.040	-18.242	1.00	28.28	A
ATOM	1854	O	ARG	A	240	-30.031	-6.814	-18.260	1.00	26.65	A
ATOM	1855	N	PHE	A	241	-28.872	-8.718	-18.502	1.00	25.31	A
ATOM	1856	CA	PHE	A	241	-27.633	-8.025	-18.822	1.00	23.21	A
ATOM	1857	CB	PHE	A	241	-26.463	-9.006	-18.705	1.00	20.31	A
ATOM	1858	CG	PHE	A	241	-25.146	-8.345	-18.481	1.00	17.38	A
ATOM	1859	CD1	PHE	A	241	-24.780	-7.948	-17.206	1.00	15.49	A
ATOM	1860	CD2	PHE	A	241	-24.297	-8.068	-19.549	1.00	17.91	A
ATOM	1861	CE1	PHE	A	241	-23.586	-7.276	-16.980	1.00	15.90	A
ATOM	1862	CE2	PHE	A	241	-23.102	-7.391	-19.330	1.00	14.47	A
ATOM	1863	CZ	PHE	A	241	-22.747	-6.997	-18.051	1.00	15.32	A
ATOM	1864	O	PHE	A	241	-27.711	-7.517	-20.271	1.00	22.81	A
ATOM	1865	N	PHE	A	241	-28.322	-8.155	-21.137	1.00	24.71	A

Figure 1 (continued 19)

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ATOM	1866	N	PRO	A	242	-27.092	-6.365	-20.556	1.00	21.66	A
ATOM	1867	CD	PRO	A	242	-26.466	-5.383	-19.664	1.00	20.82	A
ATOM	1868	CA	PRO	A	242	-27.147	-5.870	-21.936	1.00	22.07	A
ATOM	1869	CB	PRO	A	242	-26.503	-4.489	-21.849	1.00	23.09	A
ATOM	1870	CG	PRO	A	242	-25.687	-4.543	-20.635	1.00	23.90	A
ATOM	1871	C	PRO	A	242	-26.435	-6.788	-22.919	1.00	21.43	A
ATOM	1872	O	PRO	A	242	-25.517	-7.513	-22.559	1.00	21.56	A
ATOM	1873	N	ASP	A	243	-26.862	-6.730	-24.168	1.00	22.31	A
ATOM	1874	CA	ASP	A	243	-26.325	-7.544	-25.235	1.00	22.61	A
ATOM	1875	CB	ASP	A	243	-27.447	-7.789	-26.241	1.00	24.30	A
ATOM	1876	CG	ASP	A	243	-27.032	-8.665	-27.392	1.00	23.99	A
ATOM	1877	OD1	ASP	A	243	-25.841	-9.016	-27.513	1.00	23.11	A
ATOM	1878	OD2	ASP	A	243	-27.923	-9.009	-28.204	1.00	25.61	A
ATOM	1879	C	ASP	A	243	-25.164	-6.810	-25.884	1.00	22.10	A
ATOM	1880	O	ASP	A	243	-25.369	-5.814	-26.583	1.00	20.96	A
ATOM	1881	N	TYR	A	244	-23.946	-7.307	-25.690	1.00	20.24	A
ATOM	1882	CA	TYR	A	244	-22.770	-6.623	-26.253	1.00	19.79	A
ATOM	1883	CB	TYR	A	244	-21.471	-7.367	-25.865	1.00	18.34	A
ATOM	1884	CG	TYR	A	244	-21.137	-8.593	-26.702	1.00	19.53	A
ATOM	1885	CD1	TYR	A	244	-20.406	-8.482	-27.886	1.00	17.48	A
ATOM	1886	CE1	TYR	A	244	-20.127	-9.596	-28.685	1.00	19.93	A
ATOM	1887	CD2	TYR	A	244	-21.593	-9.867	-26.333	1.00	19.90	A
ATOM	1888	CE2	TYR	A	244	-21.327	-10.988	-27.129	1.00	19.80	A
ATOM	1889	CZ	TYR	A	244	-20.596	-10.862	-28.296	1.00	20.77	A
ATOM	1890	OH	TYR	A	244	-20.321	-11.983	-29.074	1.00	23.28	A
ATOM	1891	C	TYR	A	244	-22.837	-6.509	-27.775	1.00	20.37	A
ATOM	1892	O	TYR	A	244	-22.257	-5.614	-28.359	1.00	19.31	A
ATOM	1893	N	ARG	A	245	-23.534	-7.435	-28.413	1.00	19.69	A
ATOM	1894	CA	ARG	A	245	-23.627	-7.419	-29.862	1.00	22.13	A
ATOM	1895	CB	ARG	A	245	-24.410	-8.644	-30.335	1.00	22.26	A
ATOM	1896	CG	ARG	A	245	-23.819	-9.936	-29.832	1.00	24.54	A
ATOM	1897	CD	ARG	A	245	-24.691	-11.115	-30.214	1.00	27.20	A
ATOM	1898	NE	ARG	A	245	-24.296	-12.348	-29.532	1.00	28.66	A
ATOM	1899	CZ	ARG	A	245	-24.422	-12.577	-28.226	1.00	27.22	A
ATOM	1900	NH1	ARG	A	245	-24.931	-11.658	-27.413	1.00	26.49	A
ATOM	1901	NH2	ARG	A	245	-24.061	-13.756	-27.734	1.00	27.45	A
ATOM	1902	C	ARG	A	245	-24.284	-6.151	-30.393	1.00	22.87	A
ATOM	1903	O	ARG	A	245	-23.999	-5.734	-31.526	1.00	23.81	A
ATOM	1904	N	ARG	A	246	-25.168	-5.559	-29.592	1.00	22.53	A
ATOM	1905	CA	ARG	A	246	-25.866	-4.326	-29.978	1.00	23.83	A
ATOM	1906	CB	ARG	A	246	-27.271	-4.311	-29.361	1.00	23.77	A
ATOM	1907	CG	ARG	A	246	-28.060	-5.575	-29.729	1.00	27.25	A
ATOM	1908	CD	ARG	A	246	-29.543	-5.486	-29.396	1.00	29.82	A
ATOM	1909	NE	ARG	A	246	-30.202	-4.515	-30.263	1.00	32.86	A
ATOM	1910	CZ	ARG	A	246	-31.509	-4.274	-30.246	1.00	34.97	A
ATOM	1911	NH1	ARG	A	246	-32.296	-4.935	-29.410	1.00	35.99	A
ATOM	1912	NH2	ARG	A	246	-32.030	-3.375	-31.071	1.00	36.57	A
ATOM	1913	C	ARG	A	246	-25.093	-3.074	-29.554	1.00	22.99	A
ATOM	1914	O	ARG	A	246	-25.477	-1.950	-29.900	1.00	23.88	A
ATOM	1915	N	VAL	A	247	-24.027	-3.274	-28.773	1.00	21.04	A
ATOM	1916	CA	VAL	A	247	-23.177	-2.178	-28.299	1.00	20.18	A
ATOM	1917	CB	VAL	A	247	-22.685	-2.447	-26.850	1.00	19.13	A
ATOM	1918	CG1	VAL	A	247	-21.670	-1.393	-26.413	1.00	20.39	A
ATOM	1919	CG2	VAL	A	247	-23.885	-2.440	-25.907	1.00	21.24	A
ATOM	1920	C	VAL	A	247	-21.979	-1.976	-29.241	1.00	19.85	A
ATOM	1921	O	VAL	A	247	-21.472	-0.844	-29.390	1.00	20.50	A
ATOM	1922	N	LEU	A	248	-21.516	-3.048	-29.877	1.00	19.31	A
ATOM	1923	CA	LEU	A	248	-20.397	-2.896	-30.804	1.00	21.46	A
ATOM	1924	CB	LEU	A	248	-20.015	-4.239	-31.435	1.00	23.15	A
ATOM	1925	CG	LEU	A	248	-19.568	-5.316	-30.439	1.00	23.14	A
ATOM	1926	CD1	LEU	A	248	-19.300	-6.602	-31.217	1.00	26.15	A
ATOM	1927	CD2	LEU	A	248	-18.337	-4.866	-29.663	1.00	24.04	A
ATOM	1928	C	LEU	A	248	-20.810	-1.839	-31.923	1.00	22.45	A
ATOM	1929	O	LEU	A	248	-21.902	-2.054	-32.474	1.00	22.72	A
ATOM	1930	N	PRO	A	249	-19.946	-0.977	-32.273	1.00	21.88	A
ATOM	1931	CD	PRO	A	249	-18.668	-0.598	-31.642	1.00	20.48	A
ATOM	1932	CA	PRO	A	249	-20.321	-0.052	-33.353	1.00	23.12	A
ATOM	1933	CB	PRO	A	249	-19.090	0.843	-33.496	1.00	23.55	A
ATOM	1934	CG	PRO	A	249	-18.466	0.807	-32.149	1.00	22.18	A
ATOM	1935	C	PRO	A	249	-20.613	-0.821	-34.643	1.00	25.18	A
ATOM	1936	O	PRO	A	249	-19.874	-1.745	-35.018	1.00	25.69	A
ATOM	1937	N	LYS	A	250	-21.675	-0.416	-35.333	1.00	26.79	A
ATOM	1938	CA	LYS	A	250	-22.112	-1.071	-36.567	1.00	30.40	A
ATOM	1939	CB	LYS	A	250	-23.408	-0.429	-37.065	1.00	31.64	A
ATOM	1940	CG	LYS	A	250	-24.527	-0.363	-36.043	1.00	36.92	A
ATOM	1941	CD	LYS	A	250	-25.774	0.328	-36.638	1.00	40.37	A
ATOM	1942	CE	LYS	A	250	-25.511	1.793	-37.053	1.00	41.65	A
ATOM	1943	NZ	LYS	A	250	-26.750	2.478	-37.569	1.00	42.08	A
ATOM	1944	C	LYS	A	250	-21.121	-1.074	-37.714	1.00	30.98	A
ATOM	1945	O	LYS	A	250	-20.828	-2.113	-38.296	1.00	32.45	A
ATOM	1946	N	ASN	A	251	-20.612	0.098	-38.055	1.00	31.28	A
ATOM	1947	CA	ASN	A	251	-19.680	0.188	-39.161	1.00	32.02	A
ATOM	1948	CB	ASN	A	251	-20.420	0.641	-40.431	1.00	34.75	A
ATOM	1949	CG	ASN	A	251	-21.586	-0.287	-40.805	1.00	37.52	A
ATOM	1950	OD1	ASN	A	251	-22.755	0.120	-40.783	1.00	39.85	A
ATOM	1951	ND2	ASN	A	251	-21.268	-1.535	-41.154	1.00	38.31	A
ATOM	1952	C	ASN	A	251	-18.563	1.164	-38.809	1.00	30.42	A
ATOM	1953	O	ASN	A	251	-18.527	2.299	-39.297	1.00	31.94	A
ATOM	1954	N	PRO	A	252	-17.649	0.734	-37.928	1.00	28.72	A
ATOM	1955	CD	PRO	A	252	-17.660	-0.563	-37.218	1.00	27.35	A
ATOM	1956	CA	PRO	A	252	-16.517	1.563	-37.492	1.00	27.89	A
ATOM	1957	CB	PRO	A	252	-16.132	0.917	-36.167	1.00	26.42	A
ATOM	1958	CG	PRO	A	252	-16.328	-0.561	-36.468	1.00	27.43	A
ATOM	1959	C	PRO	A	252	-15.410	1.473	-38.539	1.00	29.12	A
ATOM	1960	O	PRO	A	252	-14.323	0.959	-38.263	1.00	29.62	A
ATOM	1961	N	ASP	A	253	-15.716	2.003	-39.723	1.00	30.27	A
ATOM	1962	CA	ASP	A	253	-14.869	1.991	-40.920	1.00	31.73	A
ATOM	1963	CB	ASP	A	253	-15.625	2.669	-42.079	1.00	35.32	A
ATOM	1964	CG	ASP	A	253	-15.798	4.184	-41.878	1.00	39.92	A
ATOM	1965	OD1	ASP	A	253	-16.335	4.607	-40.819	1.00	42.78	A

Figure 1 (continued 20)

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ATOM	1966	OD2	ASP	A	253	-15.400	4.962	-42.784	1.00	41.27	A
ATOM	1967	C	ASP	A	253	-13.467	2.586	-40.870	1.00	30.28	A
ATOM	1968	O	ASP	A	253	-12.578	2.126	-41.600	1.00	31.43	A
ATOM	1969	N	LYS	A	254	-13.277	3.606	-40.039	1.00	27.06	A
ATOM	1970	CA	LYS	A	254	-11.991	4.285	-39.932	1.00	24.92	A
ATOM	1971	CB	LYS	A	254	-12.232	5.728	-39.494	1.00	24.91	A
ATOM	1972	CG	LYS	A	254	-13.148	6.522	-40.421	1.00	27.11	A
ATOM	1973	CD	LYS	A	254	-13.379	7.918	-39.844	1.00	29.21	A
ATOM	1974	CE	LYS	A	254	-14.184	8.777	-40.825	1.00	32.00	A
ATOM	1975	NZ	LYS	A	254	-15.470	8.129	-41.185	1.00	34.43	A
ATOM	1976	C	LYS	A	254	-11.094	3.553	-38.930	1.00	22.15	A
ATOM	1977	O	LYS	A	254	-11.328	3.610	-37.730	1.00	22.88	A
ATOM	1978	N	HIS	A	255	-10.067	2.884	-39.434	1.00	21.10	A
ATOM	1979	CA	HIS	A	255	-9.165	2.101	-38.598	1.00	21.30	A
ATOM	1980	CB	HIS	A	255	-8.939	0.721	-39.214	1.00	24.75	A
ATOM	1981	CG	HIS	A	255	-10.171	-0.127	-39.294	1.00	26.36	A
ATOM	1982	CD2	HIS	A	255	-10.391	-1.313	-39.905	1.00	28.26	A
ATOM	1983	ND1	HIS	A	255	-11.359	0.219	-38.684	1.00	29.22	A
ATOM	1984	CE1	HIS	A	255	-12.261	-0.718	-38.922	1.00	29.44	A
ATOM	1985	NE2	HIS	A	255	-11.699	-1.658	-39.660	1.00	31.29	A
ATOM	1986	C	HIS	A	255	-7.798	2.727	-38.381	1.00	20.47	A
ATOM	1987	O	HIS	A	255	-7.045	2.966	-39.331	1.00	19.05	A
ATOM	1988	N	LEU	A	256	-7.449	2.930	-37.120	1.00	18.43	A
ATOM	1989	CA	LEU	A	256	-6.148	3.491	-36.778	1.00	18.02	A
ATOM	1990	CB	LEU	A	256	-6.351	4.753	-35.927	1.00	19.89	A
ATOM	1991	CG	LEU	A	256	-5.142	5.472	-35.324	1.00	22.32	A
ATOM	1992	CD1	LEU	A	256	-5.493	6.944	-35.096	1.00	24.64	A
ATOM	1993	CD2	LEU	A	256	-4.737	4.798	-34.007	1.00	23.40	A
ATOM	1994	C	LEU	A	256	-5.368	2.452	-35.962	1.00	18.20	A
ATOM	1995	O	LEU	A	256	-5.921	1.857	-35.042	1.00	17.77	A
ATOM	1996	N	GLU	A	257	-4.099	2.224	-36.298	1.00	16.89	A
ATOM	1997	CA	GLU	A	257	-3.295	1.292	-35.505	1.00	17.61	A
ATOM	1998	CB	GLU	A	257	-2.702	0.186	-36.378	1.00	19.65	A
ATOM	1999	CG	GLU	A	257	-1.850	-0.790	-35.585	1.00	25.47	A
ATOM	2000	CD	GLU	A	257	-1.391	-1.990	-36.398	1.00	28.58	A
ATOM	2001	OE1	GLU	A	257	-0.339	-2.592	-36.024	1.00	30.83	A
ATOM	2002	OE2	GLU	A	257	-2.089	-2.333	-37.394	1.00	26.86	A
ATOM	2003	C	GLU	A	257	-2.182	2.113	-34.861	1.00	17.45	A
ATOM	2004	O	GLU	A	257	-1.570	2.963	-35.515	1.00	16.51	A
ATOM	2005	N	ALA	A	258	-1.932	1.863	-33.579	1.00	17.17	A
ATOM	2006	CA	ALA	A	258	-0.906	2.593	-32.830	1.00	17.02	A
ATOM	2007	CB	ALA	A	258	-1.584	3.719	-32.020	1.00	18.18	A
ATOM	2008	C	ALA	A	258	-0.172	1.666	-31.864	1.00	18.03	A
ATOM	2009	O	ALA	A	258	-0.738	0.663	-31.398	1.00	17.35	A
ATOM	2010	N	GLY	A	259	1.085	2.001	-31.571	1.00	16.83	A
ATOM	2011	CA	GLY	A	259	1.860	1.248	-30.598	1.00	16.02	A
ATOM	2012	C	GLY	A	259	1.145	1.382	-29.257	1.00	16.37	A
ATOM	2013	O	GLY	A	259	0.829	2.476	-28.834	1.00	15.32	A
ATOM	2014	N	CYS	A	260	0.894	0.270	-28.576	1.00	14.83	A
ATOM	2015	CA	CYS	A	260	0.143	0.338	-27.323	1.00	14.73	A
ATOM	2016	CB	CYS	A	260	-0.107	-1.069	-26.807	1.00	13.90	A
ATOM	2017	SG	CYS	A	260	-1.234	-1.099	-25.368	1.00	18.12	A
ATOM	2018	C	CYS	A	260	0.806	1.179	-26.253	1.00	14.83	A
ATOM	2019	O	CYS	A	260	0.159	2.047	-25.640	1.00	15.46	A
ATOM	2020	N	ASP	A	261	2.096	0.921	-26.017	1.00	15.27	A
ATOM	2021	CA	ASP	A	261	2.834	1.655	-24.977	1.00	17.33	A
ATOM	2022	CB	ASP	A	261	4.276	1.123	-24.801	1.00	18.87	A
ATOM	2023	CG	ASP	A	261	5.188	2.109	-24.002	1.00	25.56	A
ATOM	2024	OD1	ASP	A	261	5.948	2.946	-24.607	1.00	27.19	A
ATOM	2025	OD2	ASP	A	261	5.128	2.056	-22.758	1.00	23.92	A
ATOM	2026	C	ASP	A	261	2.924	3.126	-25.321	1.00	15.30	A
ATOM	2027	O	ASP	A	261	2.689	3.977	-24.457	1.00	16.28	A
ATOM	2028	N	LEU	A	262	3.263	3.435	-26.566	1.00	15.05	A
ATOM	2029	CA	LEU	A	262	3.379	4.835	-26.940	1.00	14.87	A
ATOM	2030	CB	LEU	A	262	3.900	4.980	-28.365	1.00	16.84	A
ATOM	2031	CG	LEU	A	262	5.392	4.695	-28.564	1.00	19.33	A
ATOM	2032	CD1	LEU	A	262	5.705	4.835	-30.069	1.00	20.64	A
ATOM	2033	CD2	LEU	A	262	6.233	5.673	-27.721	1.00	19.45	A
ATOM	2034	C	LEU	A	262	2.041	5.563	-26.782	1.00	15.27	A
ATOM	2035	O	LEU	A	262	2.003	6.712	-26.332	1.00	15.81	A
ATOM	2036	N	LEU	A	263	0.949	4.912	-27.161	1.00	13.33	A
ATOM	2037	CA	LEU	A	263	-0.352	5.560	-26.991	1.00	13.53	A
ATOM	2038	CB	LEU	A	263	-1.447	4.721	-27.673	1.00	13.61	A
ATOM	2039	CG	LEU	A	263	-2.885	5.243	-27.627	1.00	16.53	A
ATOM	2040	CD1	LEU	A	263	-2.965	6.612	-28.293	1.00	17.32	A
ATOM	2041	CD2	LEU	A	263	-3.785	4.257	-28.319	1.00	15.91	A
ATOM	2042	C	LEU	A	263	-0.658	5.736	-25.491	1.00	14.38	A
ATOM	2043	O	LEU	A	263	-1.177	6.774	-25.064	1.00	13.47	A
ATOM	2044	N	LYS	A	264	-0.372	4.719	-24.680	1.00	13.04	A
ATOM	2045	CA	LYS	A	264	-0.655	4.778	-23.255	1.00	14.11	A
ATOM	2046	CB	LYS	A	264	-0.299	3.420	-22.644	1.00	15.66	A
ATOM	2047	CG	LYS	A	264	-0.539	3.304	-21.166	1.00	22.39	A
ATOM	2048	CD	LYS	A	264	-0.002	1.952	-20.693	1.00	25.24	A
ATOM	2049	CE	LYS	A	264	-0.624	0.789	-21.454	1.00	28.82	A
ATOM	2050	NZ	LYS	A	264	-0.186	-0.554	-20.920	1.00	32.53	A
ATOM	2051	C	LYS	A	264	0.110	5.920	-22.559	1.00	13.53	A
ATOM	2052	O	LYS	A	264	-0.474	6.700	-21.798	1.00	13.19	A
ATOM	2053	N	GLN	A	265	1.397	6.058	-22.861	1.00	12.97	A
ATOM	2054	CA	GLN	A	265	2.167	7.097	-22.192	1.00	13.73	A
ATOM	2055	CB	GLN	A	265	3.668	6.889	-22.418	1.00	14.32	A
ATOM	2056	CG	GLN	A	265	4.187	5.506	-21.997	1.00	15.83	A
ATOM	2057	CD	GLN	A	265	3.603	5.004	-20.674	1.00	16.85	A
ATOM	2058	OE1	GLN	A	265	3.288	5.773	-19.777	1.00	18.55	A
ATOM	2059	NE2	GLN	A	265	3.473	3.687	-20.551	1.00	19.72	A
ATOM	2060	C	GLN	A	265	1.789	8.491	-22.685	1.00	13.91	A
ATOM	2061	O	GLN	A	265	1.882	9.454	-21.921	1.00	14.00	A
ATOM	2062	N	ALA	A	266	1.367	8.598	-23.947	1.00	12.99	A
ATOM	2063	CA	ALA	A	266	0.949	9.897	-24.477	1.00	12.33	A
ATOM	2064	CB	ALA	A	266	0.735	9.820	-25.983	1.00	13.59	A
ATOM	2065	C	ALA	A	266	-0.356	10.311	-23.760	1.00	14.35	A

Figure 1 (continued 21)

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ATOM	2066	O	ALA	A	266	-0.533	11.459	-23.384	1.00	12.81	A
ATOM	2067	N	PHE	A	267	-1.264	9.349	-23.570	1.00	12.67	A
ATOM	2068	CA	PHE	A	267	-2.497	9.629	-22.832	1.00	14.64	A
ATOM	2069	CB	PHE	A	267	-3.412	8.384	-22.796	1.00	14.10	A
ATOM	2070	CG	PHE	A	267	-4.587	8.456	-23.724	1.00	17.70	A
ATOM	2071	CD1	PHE	A	267	-5.889	8.629	-23.221	1.00	16.72	A
ATOM	2072	CD2	PHE	A	267	-4.418	8.320	-25.085	1.00	16.56	A
ATOM	2073	CE1	PHE	A	267	-6.996	8.726	-24.090	1.00	18.75	A
ATOM	2074	CE2	PHE	A	267	-5.546	8.387	-25.986	1.00	17.43	A
ATOM	2075	CZ	PHE	A	267	-6.830	8.592	-25.468	1.00	18.69	A
ATOM	2076	C	PHE	A	267	-2.183	10.001	-21.400	1.00	13.98	A
ATOM	2077	O	PHE	A	267	-2.749	10.943	-20.853	1.00	13.44	A
ATOM	2078	N	ALA	A	268	-1.294	9.225	-20.777	1.00	13.32	A
ATOM	2079	CA	ALA	A	268	-0.945	9.470	-19.386	1.00	13.98	A
ATOM	2080	CB	ALA	A	268	-0.017	8.371	-18.892	1.00	13.57	A
ATOM	2081	C	ALA	A	268	-0.312	10.844	-19.175	1.00	11.09	A
ATOM	2082	O	ALA	A	268	-0.648	11.560	-18.212	1.00	12.76	A
ATOM	2083	N	ARG	A	269	0.568	11.264	-20.087	1.00	10.81	A
ATOM	2084	CA	ARG	A	269	1.206	12.564	-19.928	1.00	9.72	A
ATOM	2085	CB	ARG	A	269	2.418	12.695	-20.883	1.00	10.65	A
ATOM	2086	CG	ARG	A	269	3.640	11.953	-20.390	1.00	10.06	A
ATOM	2087	CD	ARG	A	269	4.892	12.362	-21.249	1.00	10.44	A
ATOM	2088	NE	ARG	A	269	4.685	12.077	-22.658	1.00	9.73	A
ATOM	2089	CZ	ARG	A	269	4.963	10.922	-23.254	1.00	9.84	A
ATOM	2090	NH1	ARG	A	269	5.499	9.908	-22.580	1.00	11.65	A
ATOM	2091	NH2	ARG	A	269	4.653	10.760	-24.520	1.00	10.88	A
ATOM	2092	C	ARG	A	269	0.217	13.699	-20.230	1.00	10.56	A
ATOM	2093	O	ARG	A	269	0.169	14.656	-19.489	1.00	11.75	A
ATOM	2094	N	ALA	A	270	-0.558	13.569	-21.309	1.00	9.54	A
ATOM	2095	CA	ALA	A	270	-1.515	14.637	-21.642	1.00	10.89	A
ATOM	2096	CB	ALA	A	270	-2.260	14.289	-22.911	1.00	13.90	A
ATOM	2097	C	ALA	A	270	-2.566	14.807	-20.483	1.00	11.27	A
ATOM	2098	O	ALA	A	270	-2.874	15.950	-20.153	1.00	12.70	A
ATOM	2099	N	ALA	A	271	-2.903	13.697	-19.871	1.00	13.03	A
ATOM	2100	CA	ALA	A	271	-3.876	13.755	-18.758	1.00	13.13	A
ATOM	2101	CB	ALA	A	271	-4.215	12.366	-18.293	1.00	12.98	A
ATOM	2102	C	ALA	A	271	-3.481	14.622	-17.569	1.00	12.80	A
ATOM	2103	O	ALA	A	271	-4.354	15.128	-16.831	1.00	12.02	A
ATOM	2104	N	ILE	A	272	-2.177	14.869	-17.385	1.00	11.81	A
ATOM	2105	CA	ILE	A	272	-1.711	15.689	-16.290	1.00	10.77	A
ATOM	2106	CB	ILE	A	272	-0.166	15.743	-16.339	1.00	10.82	A
ATOM	2107	CG2	ILE	A	272	0.362	16.726	-15.319	1.00	12.90	A
ATOM	2108	CG1	ILE	A	272	0.353	14.310	-16.155	1.00	10.24	A
ATOM	2109	CD1	ILE	A	272	1.872	14.133	-16.554	1.00	12.64	A
ATOM	2110	C	ILE	A	272	-2.287	17.132	-16.343	1.00	11.14	A
ATOM	2111	O	ILE	A	272	-2.512	17.770	-15.302	1.00	13.87	A
ATOM	2112	N	LEU	A	273	-2.507	17.638	-17.560	1.00	11.27	A
ATOM	2113	CA	LEU	A	273	-3.035	18.998	-17.702	1.00	11.91	A
ATOM	2114	CB	LEU	A	273	-2.145	19.857	-18.640	1.00	11.25	A
ATOM	2115	CG	LEU	A	273	-0.698	19.888	-18.117	1.00	12.82	A
ATOM	2116	CD1	LEU	A	273	0.147	20.788	-19.043	1.00	14.39	A
ATOM	2117	CD2	LEU	A	273	-0.605	20.368	-16.660	1.00	13.33	A
ATOM	2118	C	LEU	A	273	-4.479	19.034	-18.155	1.00	13.42	A
ATOM	2119	O	LEU	A	273	-4.918	20.032	-18.737	1.00	13.16	A
ATOM	2120	N	SER	A	274	-5.185	17.936	-17.879	1.00	13.18	A
ATOM	2121	CA	SER	A	274	-6.625	17.884	-18.193	1.00	16.03	A
ATOM	2122	CB	SER	A	274	-7.040	16.461	-18.570	1.00	15.17	A
ATOM	2123	CG	SER	A	274	-6.960	15.560	-17.484	1.00	16.66	A
ATOM	2124	C	SER	A	274	-7.363	18.365	-16.933	1.00	15.64	A
ATOM	2125	O	SER	A	274	-6.734	18.682	-15.911	1.00	17.51	A
ATOM	2126	N	ASN	A	275	-8.696	18.484	-16.988	1.00	14.62	A
ATOM	2127	CA	ASN	A	275	-9.397	18.935	-15.774	1.00	17.24	A
ATOM	2128	CB	ASN	A	275	-10.872	19.209	-16.082	1.00	16.46	A
ATOM	2129	CG	ASN	A	275	-11.590	19.909	-14.923	1.00	18.43	A
ATOM	2130	OD1	ASN	A	275	-11.704	19.358	-13.827	1.00	22.10	A
ATOM	2131	ND2	ASN	A	275	-12.067	21.138	-15.170	1.00	18.70	A
ATOM	2132	C	ASN	A	275	-9.307	17.879	-14.662	1.00	18.08	A
ATOM	2133	O	ASN	A	275	-9.747	16.752	-14.843	1.00	17.91	A
ATOM	2134	N	GLU	A	276	-8.718	18.235	-13.523	1.00	21.67	A
ATOM	2135	CA	GLU	A	276	-8.539	17.290	-12.401	1.00	25.21	A
ATOM	2136	CB	GLU	A	276	-7.902	17.993	-11.189	1.00	30.38	A
ATOM	2137	CG	GLU	A	276	-6.672	18.817	-11.475	1.00	37.32	A
ATOM	2138	CD	GLU	A	276	-5.401	17.997	-11.551	1.00	42.05	A
ATOM	2139	OE1	GLU	A	276	-5.122	17.211	-10.603	1.00	44.93	A
ATOM	2140	OE2	GLU	A	276	-4.667	18.154	-12.553	1.00	45.14	A
ATOM	2141	C	GLU	A	276	-9.796	16.578	-11.907	1.00	26.06	A
ATOM	2142	O	GLU	A	276	-9.724	15.425	-11.457	1.00	24.42	A
ATOM	2143	N	LYS	A	277	-10.946	17.254	-11.984	1.00	25.49	A
ATOM	2144	CA	LYS	A	277	-12.218	16.681	-11.525	1.00	27.23	A
ATOM	2145	CB	LYS	A	277	-13.203	17.806	-11.157	1.00	29.01	A
ATOM	2146	CG	LYS	A	277	-12.699	18.790	-10.106	1.00	33.53	A
ATOM	2147	CD	LYS	A	277	-12.724	18.215	-8.698	1.00	36.20	A
ATOM	2148	CE	LYS	A	277	-12.225	19.257	-7.698	1.00	37.26	A
ATOM	2149	NZ	LYS	A	277	-12.511	18.878	-6.273	1.00	39.68	A
ATOM	2150	C	LYS	A	277	-12.884	15.775	-12.562	1.00	25.59	A
ATOM	2151	O	LYS	A	277	-13.731	14.943	-12.220	1.00	25.69	A
ATOM	2152	N	PHE	A	278	-12.498	15.921	-13.825	1.00	24.84	A
ATOM	2153	CA	PHE	A	278	-13.092	15.122	-14.896	1.00	23.67	A
ATOM	2154	CB	PHE	A	278	-14.380	15.816	-15.313	1.00	25.91	A
ATOM	2155	CG	PHE	A	278	-15.369	14.929	-15.984	1.00	29.29	A
ATOM	2156	CD1	PHE	A	278	-15.276	13.538	-15.875	1.00	30.58	A
ATOM	2157	CD2	PHE	A	278	-16.425	15.485	-16.705	1.00	30.56	A
ATOM	2158	CE1	PHE	A	278	-16.220	12.710	-16.471	1.00	32.00	A
ATOM	2159	CE2	PHE	A	278	-17.383	14.658	-17.310	1.00	31.23	A
ATOM	2160	CZ	PHE	A	278	-17.278	13.270	-17.191	1.00	33.81	A
ATOM	2161	C	PHE	A	278	-12.076	15.063	-16.050	1.00	21.94	A
ATOM	2162	O	PHE	A	278	-12.137	15.874	-16.575	1.00	21.84	A
ATOM	2163	N	ARG	A	279	-11.154	14.096	-15.989	1.00	19.13	A
ATOM	2164	CA	ARG	A	279	-10.063	14.036	-16.962	1.00	18.33	A
ATOM	2165	CB	ARG	A	279	-8.844	13.272	-16.376	1.00	18.78	A

Figure 1 (continued 22)

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ATOM	2166	CG	ARG	A	279	-8.186	13.898	-15.146	1.00	23.64	A
ATOM	2167	CD	ARG	A	279	-6.825	13.215	-14.864	1.00	26.45	A
ATOM	2168	NE	ARG	A	279	-6.393	13.464	-13.493	1.00	31.51	A
ATOM	2169	CZ	ARG	A	279	-5.871	14.612	-13.074	1.00	33.69	A
ATOM	2170	NH1	ARG	A	279	-5.708	15.616	-13.934	1.00	35.31	A
ATOM	2171	NH2	ARG	A	279	-5.529	14.763	-11.792	1.00	33.02	A
ATOM	2172	C	ARG	A	279	-10.359	13.458	-18.314	1.00	14.43	A
ATOM	2173	O	ARG	A	279	-10.674	12.294	-18.433	1.00	16.83	A
ATOM	2174	N	GLY	A	280	-10.222	14.291	-19.333	1.00	14.30	A
ATOM	2175	CA	GLY	A	280	-10.420	13.855	-20.696	1.00	13.40	A
ATOM	2176	C	GLY	A	280	-9.408	14.511	-21.632	1.00	12.18	A
ATOM	2177	O	GLY	A	280	-8.837	15.565	-21.311	1.00	13.28	A
ATOM	2178	N	VAL	A	281	-9.193	13.896	-22.795	1.00	13.04	A
ATOM	2179	CA	VAL	A	281	-8.254	14.440	-23.796	1.00	12.38	A
ATOM	2180	CB	VAL	A	281	-6.960	13.531	-23.909	1.00	13.51	A
ATOM	2181	CG1	VAL	A	281	-6.103	13.679	-22.671	1.00	12.12	A
ATOM	2182	CG2	VAL	A	281	-7.362	12.090	-24.098	1.00	15.36	A
ATOM	2183	C	VAL	A	281	-8.927	14.482	-25.165	1.00	12.53	A
ATOM	2184	O	VAL	A	281	-9.866	13.716	-25.457	1.00	13.70	A
ATOM	2185	N	ARG	A	282	-8.453	15.380	-26.026	1.00	11.74	A
ATOM	2186	CA	ARG	A	282	-8.987	15.486	-27.364	1.00	13.08	A
ATOM	2187	CB	ARG	A	282	-9.165	16.947	-27.763	1.00	16.93	A
ATOM	2188	CG	ARG	A	282	-9.831	17.086	-29.125	1.00	25.93	A
ATOM	2189	CD	ARG	A	282	-11.067	18.017	-29.069	1.00	33.09	A
ATOM	2190	NE	ARG	A	282	-11.959	17.716	-27.940	1.00	37.56	A
ATOM	2191	CZ	ARG	A	282	-13.099	17.025	-28.030	1.00	38.42	A
ATOM	2192	NH1	ARG	A	282	-13.519	16.552	-29.200	1.00	38.59	A
ATOM	2193	NH2	ARG	A	282	-13.822	16.805	-26.940	1.00	38.91	A
ATOM	2194	C	ARG	A	282	-8.029	14.816	-28.330	1.00	14.43	A
ATOM	2195	O	ARG	A	282	-6.815	15.031	-28.216	1.00	16.20	A
ATOM	2196	N	LEU	A	283	-8.566	14.022	-29.267	1.00	12.40	A
ATOM	2197	CA	LEU	A	283	-7.754	13.341	-30.279	1.00	13.04	A
ATOM	2198	CB	LEU	A	283	-8.052	11.840	-30.387	1.00	14.68	A
ATOM	2199	CG	LEU	A	283	-7.290	10.870	-29.488	1.00	17.14	A
ATOM	2200	CD1	LEU	A	283	-7.408	11.334	-28.017	1.00	18.12	A
ATOM	2201	CD2	LEU	A	283	-7.795	9.422	-29.716	1.00	17.55	A
ATOM	2202	C	LEU	A	283	-8.039	13.920	-31.638	1.00	15.68	A
ATOM	2203	O	LEU	A	283	-9.192	14.041	-32.036	1.00	15.80	A
ATOM	2204	N	TYR	A	284	-6.988	14.308	-32.338	1.00	13.31	A
ATOM	2205	CA	TYR	A	284	-7.186	14.776	-33.696	1.00	14.87	A
ATOM	2206	CB	TYR	A	284	-6.561	16.144	-33.942	1.00	14.87	A
ATOM	2207	CG	TYR	A	284	-7.063	16.684	-35.265	1.00	16.70	A
ATOM	2208	CD1	TYR	A	284	-8.155	17.562	-35.312	1.00	18.02	A
ATOM	2209	CE1	TYR	A	284	-8.709	17.978	-36.542	1.00	19.42	A
ATOM	2210	CD2	TYR	A	284	-6.532	16.232	-36.466	1.00	16.24	A
ATOM	2211	CE2	TYR	A	284	-7.077	16.638	-37.685	1.00	18.82	A
ATOM	2212	CZ	TYR	A	284	-8.165	17.514	-37.713	1.00	19.97	A
ATOM	2213	OH	TYR	A	284	-8.692	17.919	-38.933	1.00	20.44	A
ATOM	2214	C	TYR	A	284	-6.517	13.731	-34.561	1.00	14.90	A
ATOM	2215	O	TYR	A	284	-5.293	13.519	-34.503	1.00	15.97	A
ATOM	2216	N	VAL	A	285	-7.320	13.050	-35.369	1.00	14.02	A
ATOM	2217	CA	VAL	A	285	-6.768	12.007	-36.209	1.00	14.58	A
ATOM	2218	CB	VAL	A	285	-7.728	10.797	-36.264	1.00	16.41	A
ATOM	2219	CG1	VAL	A	285	-7.087	9.678	-37.030	1.00	19.28	A
ATOM	2220	CG2	VAL	A	285	-8.053	10.335	-34.836	1.00	17.87	A
ATOM	2221	C	VAL	A	285	-6.566	12.520	-37.613	1.00	13.95	A
ATOM	2222	O	VAL	A	285	-7.463	13.109	-38.191	1.00	16.55	A
ATOM	2223	N	SER	A	286	-5.376	12.297	-38.168	1.00	13.98	A
ATOM	2224	CA	SER	A	286	-5.094	12.724	-39.555	1.00	13.75	A
ATOM	2225	CB	SER	A	286	-4.453	14.123	-39.576	1.00	15.23	A
ATOM	2226	CG	SER	A	286	-3.165	14.108	-38.984	1.00	16.02	A
ATOM	2227	C	SER	A	286	-4.198	11.659	-40.201	1.00	15.02	A
ATOM	2228	O	SER	A	286	-3.859	10.670	-39.558	1.00	15.90	A
ATOM	2229	N	GLU	A	287	-3.806	11.824	-41.465	1.00	16.50	A
ATOM	2230	CA	GLU	A	287	-3.006	10.788	-42.132	1.00	17.09	A
ATOM	2231	CB	GLU	A	287	-2.655	11.245	-43.568	1.00	20.13	A
ATOM	2232	CG	GLU	A	287	-2.338	10.108	-44.526	1.00	25.94	A
ATOM	2233	CD	GLU	A	287	-3.594	9.464	-45.178	1.00	31.11	A
ATOM	2234	OE1	GLU	A	287	-4.753	9.927	-44.995	1.00	33.30	A
ATOM	2235	OE2	GLU	A	287	-3.410	8.466	-45.909	1.00	36.38	A
ATOM	2236	C	GLU	A	287	-1.752	10.371	-41.363	1.00	17.84	A
ATOM	2237	O	GLU	A	287	-0.845	11.172	-41.104	1.00	16.79	A
ATOM	2238	N	ASN	A	288	-1.734	9.100	-40.955	1.00	15.55	A
ATOM	2239	CA	ASN	A	288	-0.648	8.524	-40.188	1.00	15.15	A
ATOM	2240	CB	ASN	A	288	0.548	8.265	-41.097	1.00	18.14	A
ATOM	2241	CG	ASN	A	288	0.272	7.178	-42.139	1.00	19.57	A
ATOM	2242	OD1	ASN	A	288	0.911	7.151	-43.202	1.00	24.08	A
ATOM	2243	ND2	ASN	A	288	-0.643	6.263	-43.837	1.00	15.66	A
ATOM	2244	C	ASN	A	288	-0.221	9.333	-38.969	1.00	14.72	A
ATOM	2245	O	ASN	A	288	0.933	9.275	-38.548	1.00	15.32	A
ATOM	2246	N	GLN	A	289	-1.149	10.083	-38.380	1.00	12.97	A
ATOM	2247	CA	GLN	A	289	-0.790	10.867	-37.209	1.00	13.76	A
ATOM	2248	CB	GLN	A	289	-0.352	12.282	-37.632	1.00	14.58	A
ATOM	2249	CG	GLN	A	289	0.205	13.125	-36.486	1.00	15.69	A
ATOM	2250	CD	GLN	A	289	0.526	14.534	-36.923	1.00	19.41	A
ATOM	2251	OE1	GLN	A	289	-0.299	15.468	-36.764	1.00	22.72	A
ATOM	2252	NE2	GLN	A	289	1.714	14.705	-37.504	1.00	20.35	A
ATOM	2253	C	GLN	A	289	-1.906	11.022	-36.223	1.00	15.19	A
ATOM	2254	O	GLN	A	289	-3.074	11.137	-36.603	1.00	14.85	A
ATOM	2255	N	LEU	A	290	-1.554	11.041	-34.941	1.00	13.50	A
ATOM	2256	CA	LEU	A	290	-2.559	11.268	-33.903	1.00	13.78	A
ATOM	2257	CB	LEU	A	290	-2.738	10.022	-33.017	1.00	15.99	A
ATOM	2258	CG	LEU	A	290	-3.770	10.099	-31.894	1.00	18.63	A
ATOM	2259	CD1	LEU	A	290	-5.182	10.294	-32.481	1.00	17.72	A
ATOM	2260	CD2	LEU	A	290	-3.706	8.818	-31.090	1.00	17.47	A
ATOM	2261	C	LEU	A	290	-2.022	12.403	-33.039	1.00	13.83	A
ATOM	2262	O	LEU	A	290	-0.872	12.377	-32.625	1.00	14.65	A
ATOM	2263	N	LYS	A	291	-2.864	13.395	-32.755	1.00	12.16	A
ATOM	2264	CA	LYS	A	291	-2.478	14.486	-31.879	1.00	13.66	A
ATOM	2265	CB	LYS	A	291	-2.713	15.847	-32.532	1.00	16.40	A

Figure 1 (continued 23)

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ATOM	2266	CG	LYS	A	291	-2.319	17.009	-31.620	1.00	19.58	A
ATOM	2267	CD	LYS	A	291	-2.331	18.365	-32.360	1.00	23.93	A
ATOM	2268	CE	LYS	A	291	-1.322	18.403	-33.488	1.00	28.14	A
ATOM	2269	NZ	LYS	A	291	-1.660	19.396	-34.584	1.00	31.96	A
ATOM	2270	C	LYS	A	291	-3.376	14.347	-30.667	1.00	14.91	A
ATOM	2271	O	LYS	A	291	-4.586	14.165	-30.812	1.00	16.66	A
ATOM	2272	N	ILE	A	292	-2.798	14.395	-29.480	1.00	12.63	A
ATOM	2273	CA	ILE	A	292	-3.606	14.274	-28.272	1.00	12.23	A
ATOM	2274	CB	ILE	A	292	-3.122	13.080	-27.435	1.00	10.96	A
ATOM	2275	CG2	ILE	A	292	-3.842	13.062	-26.067	1.00	11.48	A
ATOM	2276	CG1	ILE	A	292	-3.343	11.776	-28.240	1.00	13.80	A
ATOM	2277	CD1	ILE	A	292	-2.721	10.538	-27.591	1.00	15.45	A
ATOM	2278	C	ILE	A	292	-3.413	15.562	-27.478	1.00	14.22	A
ATOM	2279	O	ILE	A	292	-2.275	15.928	-27.152	1.00	14.71	A
ATOM	2280	N	THR	A	293	-4.514	16.240	-27.130	1.00	12.06	A
ATOM	2281	CA	THR	A	293	-4.395	17.489	-26.392	1.00	12.49	A
ATOM	2282	CB	THR	A	293	-4.757	18.694	-27.302	1.00	14.10	A
ATOM	2283	OG1	THR	A	293	-6.127	18.615	-27.691	1.00	20.69	A
ATOM	2284	CG2	THR	A	293	-3.957	18.676	-28.566	1.00	13.47	A
ATOM	2285	C	THR	A	293	-5.284	17.512	-25.142	1.00	13.28	A
ATOM	2286	O	THR	A	293	-6.324	16.840	-25.073	1.00	13.69	A
ATOM	2287	N	ALA	A	294	-4.817	18.231	-24.147	1.00	11.90	A
ATOM	2288	CA	ALA	A	294	-5.546	18.421	-22.880	1.00	11.99	A
ATOM	2289	CB	ALA	A	294	-4.986	17.521	-21.790	1.00	14.59	A
ATOM	2290	C	ALA	A	294	-5.443	19.858	-22.433	1.00	11.96	A
ATOM	2291	O	ALA	A	294	-4.440	20.536	-22.685	1.00	13.42	A
ATOM	2292	N	ASN	A	295	-6.472	20.330	-21.721	1.00	13.29	A
ATOM	2293	CA	ASN	A	295	-6.503	21.690	-21.209	1.00	15.53	A
ATOM	2294	CB	ASN	A	295	-7.326	22.622	-22.129	1.00	20.85	A
ATOM	2295	CG	ASN	A	295	-6.805	22.666	-23.539	1.00	23.25	A
ATOM	2296	OD1	ASN	A	295	-6.030	23.558	-23.901	1.00	29.01	A
ATOM	2297	ND2	ASN	A	295	-7.217	21.704	-24.350	1.00	25.32	A
ATOM	2298	C	ASN	A	295	-7.244	21.643	-19.881	1.00	13.79	A
ATOM	2299	O	ASN	A	295	-8.046	20.725	-19.625	1.00	14.51	A
ATOM	2300	N	ASN	A	296	-6.970	22.631	-19.048	1.00	14.40	A
ATOM	2301	CA	ASN	A	296	-7.627	22.709	-17.746	1.00	15.59	A
ATOM	2302	CB	ASN	A	296	-6.711	22.122	-16.646	1.00	15.58	A
ATOM	2303	CG	ASN	A	296	-5.444	22.935	-16.427	1.00	15.76	A
ATOM	2304	OD1	ASN	A	296	-5.394	24.114	-16.766	1.00	15.10	A
ATOM	2305	ND2	ASN	A	296	-4.415	22.304	-15.829	1.00	18.05	A
ATOM	2306	C	ASN	A	296	-8.068	24.163	-17.462	1.00	16.76	A
ATOM	2307	O	ASN	A	296	-7.770	25.094	-18.230	1.00	15.08	A
ATOM	2308	N	PRO	A	297	-8.769	24.383	-16.344	1.00	20.01	A
ATOM	2309	CD	PRO	A	297	-9.315	23.409	-15.393	1.00	21.18	A
ATOM	2310	CA	PRO	A	297	-9.225	25.747	-16.039	1.00	22.92	A
ATOM	2311	CB	PRO	A	297	-10.099	25.553	-14.792	1.00	23.25	A
ATOM	2312	CG	PRO	A	297	-10.607	24.125	-14.971	1.00	22.77	A
ATOM	2313	C	PRO	A	297	-8.127	26.786	-15.819	1.00	24.45	A
ATOM	2314	O	PRO	A	297	-8.382	28.000	-15.915	1.00	27.11	A
ATOM	2315	N	GLU	A	298	-6.919	26.306	-15.521	1.00	24.38	A
ATOM	2316	CA	GLU	A	298	-5.767	27.174	-15.283	1.00	24.08	A
ATOM	2317	CB	GLU	A	298	-4.690	26.433	-14.480	1.00	26.78	A
ATOM	2318	CG	GLU	A	298	-5.007	26.166	-12.995	1.00	33.37	A
ATOM	2319	CD	GLU	A	298	-5.908	24.952	-12.723	1.00	35.97	A
ATOM	2320	OE1	GLU	A	298	-6.051	24.608	-11.528	1.00	39.62	A
ATOM	2321	OE2	GLU	A	298	-6.473	24.342	-13.664	1.00	36.85	A
ATOM	2322	C	GLU	A	298	-5.177	27.605	-16.627	1.00	23.08	A
ATOM	2323	O	GLU	A	298	-4.175	28.329	-16.679	1.00	21.84	A
ATOM	2324	N	GLN	A	299	-5.801	27.151	-17.707	1.00	19.62	A
ATOM	2325	CA	GLN	A	299	-5.382	27.476	-19.060	1.00	20.73	A
ATOM	2326	CB	GLN	A	299	-5.146	28.988	-19.244	1.00	25.04	A
ATOM	2327	CG	GLN	A	299	-6.153	29.921	-18.590	1.00	31.94	A
ATOM	2328	CD	GLN	A	299	-5.734	31.391	-18.727	1.00	35.89	A
ATOM	2329	OE1	GLN	A	299	-5.505	31.880	-19.840	1.00	38.44	A
ATOM	2330	NE2	GLN	A	299	-5.626	32.098	-17.592	1.00	37.47	A
ATOM	2331	C	GLN	A	299	-4.089	26.767	-19.419	1.00	18.90	A
ATOM	2332	O	GLN	A	299	-3.418	27.164	-20.383	1.00	18.74	A
ATOM	2333	N	GLU	A	300	-3.720	25.771	-18.624	1.00	14.58	A
ATOM	2334	CA	GLU	A	300	-2.511	24.997	-18.951	1.00	13.30	A
ATOM	2335	CB	GLU	A	300	-2.035	24.255	-17.708	1.00	14.18	A
ATOM	2336	CG	GLU	A	300	-1.593	25.228	-16.642	1.00	12.48	A
ATOM	2337	CD	GLU	A	300	-1.279	24.555	-15.320	1.00	14.90	A
ATOM	2338	OE1	GLU	A	300	-1.927	23.543	-14.997	1.00	15.04	A
ATOM	2339	OE2	GLU	A	300	-0.394	25.073	-14.582	1.00	17.40	A
ATOM	2340	C	GLU	A	300	-2.889	24.054	-20.079	1.00	13.11	A
ATOM	2341	O	GLU	A	300	-4.065	23.715	-20.262	1.00	14.26	A
ATOM	2342	N	GLU	A	301	-1.899	23.602	-20.856	1.00	12.23	A
ATOM	2343	CA	GLU	A	301	-2.215	22.772	-22.001	1.00	13.64	A
ATOM	2344	CB	GLU	A	301	-2.406	23.648	-23.246	1.00	17.30	A
ATOM	2345	CG	GLU	A	301	-2.865	22.871	-24.488	1.00	22.48	A
ATOM	2346	CD	GLU	A	301	-3.254	23.787	-25.635	1.00	27.65	A
ATOM	2347	OE1	GLU	A	301	-2.342	24.430	-26.200	1.00	31.10	A
ATOM	2348	OE2	GLU	A	301	-4.462	23.877	-25.961	1.00	30.41	A
ATOM	2349	C	GLU	A	301	-1.105	21.789	-22.298	1.00	12.28	A
ATOM	2350	O	GLU	A	301	0.074	22.112	-22.107	1.00	12.26	A
ATOM	2351	N	ALA	A	302	-1.515	20.604	-22.734	1.00	11.02	A
ATOM	2352	CA	ALA	A	302	-0.562	19.544	-23.111	1.00	11.63	A
ATOM	2353	CB	ALA	A	302	-0.699	18.342	-22.188	1.00	12.84	A
ATOM	2354	C	ALA	A	302	-0.834	19.101	-24.550	1.00	13.62	A
ATOM	2355	O	ALA	A	302	-1.992	19.077	-25.003	1.00	15.53	A
ATOM	2356	N	GLU	A	303	0.223	18.780	-25.301	1.00	10.01	A
ATOM	2357	CA	GLU	A	303	0.026	18.255	-26.636	1.00	11.02	A
ATOM	2358	CB	GLU	A	303	0.253	19.320	-27.697	1.00	13.49	A
ATOM	2359	CG	GLU	A	303	0.127	18.797	-29.115	1.00	16.09	A
ATOM	2360	CD	GLU	A	303	0.446	19.851	-30.167	1.00	19.61	A
ATOM	2361	OE1	GLU	A	303	-0.479	20.607	-30.584	1.00	20.94	A
ATOM	2362	OE2	GLU	A	303	1.628	19.928	-30.579	1.00	18.80	A
ATOM	2363	C	GLU	A	303	1.009	17.109	-26.887	1.00	11.44	A
ATOM	2364	O	GLU	A	303	2.169	17.226	-26.550	1.00	13.57	A
ATOM	2365	N	GLU	A	304	0.513	16.006	-27.427	1.00	10.72	A

Figure 1 (continued 24)

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ATOM	2366	CA	GLU	A	304	1.385	14.866	-27.767	1.00	10.97	A
ATOM	2367	CB	GLU	A	304	0.994	13.647	-26.932	1.00	12.53	A
ATOM	2368	CG	GLU	A	304	1.248	13.808	-25.483	1.00	12.60	A
ATOM	2369	CD	GLU	A	304	2.714	13.563	-25.117	1.00	12.60	A
ATOM	2370	OE1	GLU	A	304	3.469	13.052	-25.981	1.00	12.80	A
ATOM	2371	OE2	GLU	A	304	3.069	13.867	-23.965	1.00	12.17	A
ATOM	2372	C	GLU	A	304	1.147	14.532	-29.244	1.00	12.99	A
ATOM	2373	O	GLU	A	304	-0.007	14.450	-29.672	1.00	14.60	A
ATOM	2374	N	ILE	A	305	2.205	14.349	-30.033	1.00	11.72	A
ATOM	2375	CA	ILE	A	305	1.999	13.953	-31.414	1.00	13.62	A
ATOM	2376	CB	ILE	A	305	2.631	14.950	-32.417	1.00	15.28	A
ATOM	2377	CG2	ILE	A	305	2.424	14.412	-33.857	1.00	16.72	A
ATOM	2378	CG1	ILE	A	305	1.904	16.312	-32.316	1.00	14.51	A
ATOM	2379	CD1	ILE	A	305	2.546	17.468	-33.066	1.00	19.83	A
ATOM	2380	C	ILE	A	305	2.611	12.557	-31.532	1.00	14.02	A
ATOM	2381	O	ILE	A	305	3.727	12.288	-31.012	1.00	13.98	A
ATOM	2382	N	LEU	A	306	1.859	11.651	-32.154	1.00	12.94	A
ATOM	2383	CA	LEU	A	306	2.313	10.259	-32.344	1.00	14.07	A
ATOM	2384	CB	LEU	A	306	1.444	9.265	-31.558	1.00	17.83	A
ATOM	2385	CG	LEU	A	306	1.426	9.316	-30.037	1.00	19.01	A
ATOM	2386	CD1	LEU	A	306	0.496	8.218	-29.532	1.00	21.97	A
ATOM	2387	CD2	LEU	A	306	2.844	9.079	-29.473	1.00	23.23	A
ATOM	2388	C	LEU	A	306	2.203	9.831	-33.795	1.00	14.91	A
ATOM	2389	O	LEU	A	306	1.284	10.228	-34.487	1.00	14.55	A
ATOM	2390	N	ASP	A	307	3.165	9.032	-34.271	1.00	14.49	A
ATOM	2391	CA	ASP	A	307	3.013	8.483	-35.615	1.00	16.69	A
ATOM	2392	CB	ASP	A	307	4.337	7.966	-36.168	1.00	19.50	A
ATOM	2393	CG	ASP	A	307	5.282	9.065	-36.529	1.00	22.90	A
ATOM	2394	OD1	ASP	A	307	4.830	10.194	-36.789	1.00	22.13	A
ATOM	2395	OD2	ASP	A	307	6.491	8.777	-36.579	1.00	29.27	A
ATOM	2396	C	ASP	A	307	2.109	7.266	-35.421	1.00	16.05	A
ATOM	2397	O	ASP	A	307	2.294	6.492	-34.470	1.00	16.80	A
ATOM	2398	N	VAL	A	308	1.148	7.074	-36.308	1.00	14.24	A
ATOM	2399	CA	VAL	A	308	0.244	5.918	-36.228	1.00	14.78	A
ATOM	2400	CB	VAL	A	308	-1.128	6.256	-35.539	1.00	14.59	A
ATOM	2401	CG1	VAL	A	308	-0.889	6.738	-34.086	1.00	14.50	A
ATOM	2402	CG2	VAL	A	308	-1.906	7.299	-36.330	1.00	16.78	A
ATOM	2403	C	VAL	A	308	-0.028	5.511	-37.664	1.00	15.25	A
ATOM	2404	O	VAL	A	308	0.473	6.156	-38.597	1.00	14.77	A
ATOM	2405	N	THR	A	309	-0.820	4.458	-37.849	1.00	15.22	A
ATOM	2406	CA	THR	A	309	-1.192	4.055	-39.199	1.00	16.94	A
ATOM	2407	CB	THR	A	309	-0.982	2.562	-39.446	1.00	18.38	A
ATOM	2408	OG1	THR	A	309	0.392	2.246	-39.265	1.00	20.45	A
ATOM	2409	CG2	THR	A	309	-1.399	2.210	-40.906	1.00	21.07	A
ATOM	2410	C	THR	A	309	-2.653	4.383	-39.373	1.00	16.41	A
ATOM	2411	O	THR	A	309	-3.508	3.790	-38.723	1.00	18.35	A
ATOM	2412	N	TYR	A	310	-2.936	5.346	-40.240	1.00	14.86	A
ATOM	2413	CA	TYR	A	310	-4.291	5.797	-40.505	1.00	15.78	A
ATOM	2414	CB	TYR	A	310	-4.743	6.802	-39.441	1.00	17.41	A
ATOM	2415	CG	TYR	A	310	-6.152	7.240	-39.641	1.00	18.61	A
ATOM	2416	CD1	TYR	A	310	-7.202	6.359	-39.418	1.00	20.45	A
ATOM	2417	CE1	TYR	A	310	-8.519	6.753	-39.640	1.00	22.76	A
ATOM	2418	CD2	TYR	A	310	-6.453	8.526	-40.087	1.00	20.08	A
ATOM	2419	CE2	TYR	A	310	-7.758	8.926	-40.308	1.00	20.45	A
ATOM	2420	CZ	TYR	A	310	-8.787	8.036	-40.087	1.00	22.23	A
ATOM	2421	OH	TYR	A	310	-10.077	8.431	-40.323	1.00	23.32	A
ATOM	2422	C	TYR	A	310	-4.412	6.478	-41.843	1.00	19.52	A
ATOM	2423	O	TYR	A	310	-3.625	7.372	-42.149	1.00	18.32	A
ATOM	2424	N	SER	A	311	-5.406	6.070	-42.633	1.00	20.36	A
ATOM	2425	CA	SER	A	311	-5.620	6.668	-43.951	1.00	24.14	A
ATOM	2426	CB	SER	A	311	-5.341	5.642	-45.027	1.00	24.45	A
ATOM	2427	OG	SER	A	311	-6.267	4.577	-44.882	1.00	29.21	A
ATOM	2428	C	SER	A	311	-7.028	7.222	-44.203	1.00	26.37	A
ATOM	2429	O	SER	A	311	-7.348	7.596	-45.336	1.00	30.35	A
ATOM	2430	N	GLY	A	312	-7.880	7.275	-43.196	1.00	28.49	A
ATOM	2431	CA	GLY	A	312	-9.217	7.803	-43.441	1.00	28.97	A
ATOM	2432	C	GLY	A	312	-9.365	9.320	-43.383	1.00	28.05	A
ATOM	2433	O	GLY	A	312	-8.380	10.057	-43.420	1.00	29.05	A
ATOM	2434	N	ALA	A	313	-10.607	9.794	-43.303	1.00	27.21	A
ATOM	2435	CA	ALA	A	313	-10.876	11.232	-43.199	1.00	24.74	A
ATOM	2436	CB	ALA	A	313	-12.346	11.499	-43.370	1.00	26.37	A
ATOM	2437	C	ALA	A	313	-10.436	11.749	-41.826	1.00	22.97	A
ATOM	2438	O	ALA	A	313	-10.352	10.984	-40.871	1.00	21.96	A
ATOM	2439	N	GLU	A	314	-10.168	13.043	-41.720	1.00	20.72	A
ATOM	2440	CA	GLU	A	314	-9.756	13.591	-40.439	1.00	18.80	A
ATOM	2441	CB	GLU	A	314	-9.055	14.960	-40.587	1.00	17.54	A
ATOM	2442	CG	GLU	A	314	-7.815	14.898	-41.505	1.00	16.92	A
ATOM	2443	CD	GLU	A	314	-6.990	16.211	-41.564	1.00	13.92	A
ATOM	2444	OE1	GLU	A	314	-7.488	17.275	-41.169	1.00	16.98	A
ATOM	2445	OE2	GLU	A	314	-5.833	16.145	-42.040	1.00	16.78	A
ATOM	2446	C	GLU	A	314	-10.962	13.753	-39.540	1.00	19.37	A
ATOM	2447	O	GLU	A	314	-12.103	13.914	-39.997	1.00	19.24	A
ATOM	2448	N	MET	A	315	-10.712	13.695	-38.244	1.00	17.56	A
ATOM	2449	CA	MET	A	315	-11.773	13.901	-37.273	1.00	18.80	A
ATOM	2450	CB	MET	A	315	-12.687	12.671	-37.207	1.00	20.81	A
ATOM	2451	CG	MET	A	315	-11.969	11.387	-36.964	1.00	21.30	A
ATOM	2452	SD	MET	A	315	-13.164	10.037	-36.647	1.00	27.18	A
ATOM	2453	CE	MET	A	315	-13.747	10.557	-35.201	1.00	21.45	A
ATOM	2454	C	MET	A	315	-11.181	14.209	-35.907	1.00	18.44	A
ATOM	2455	O	MET	A	315	-10.018	13.895	-35.631	1.00	17.20	A
ATOM	2456	N	GLU	A	316	-11.973	14.872	-35.075	1.00	16.93	A
ATOM	2457	CA	GLU	A	316	-11.563	15.231	-33.736	1.00	18.29	A
ATOM	2458	CB	GLU	A	316	-11.582	16.742	-33.551	1.00	21.52	A
ATOM	2459	CG	GLU	A	316	-11.083	17.217	-32.220	1.00	27.35	A
ATOM	2460	CD	GLU	A	316	-10.835	18.712	-32.236	1.00	32.67	A
ATOM	2461	OE1	GLU	A	316	-11.793	19.470	-32.520	1.00	33.72	A
ATOM	2462	OE2	GLU	A	316	-9.685	19.135	-31.984	1.00	35.34	A
ATOM	2463	C	GLU	A	316	-12.582	14.584	-32.819	1.00	17.89	A
ATOM	2464	O	GLU	A	316	-13.801	14.685	-33.042	1.00	20.54	A
ATOM	2465	N	ILE	A	317	-12.087	13.908	-31.801	1.00	14.19	A

Figure 1 (continued 25)

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ATOM	2466	CA	ILE	A	317	-12.975	13.213	-30.866	1.00	13.52	A
ATOM	2467	CB	ILE	A	317	-13.258	11.774	-31.384	1.00	14.49	A
ATOM	2468	CG2	ILE	A	317	-11.953	10.954	-31.387	1.00	12.63	A
ATOM	2469	CG1	ILE	A	317	-14.247	11.046	-30.452	1.00	14.36	A
ATOM	2470	CD1	ILE	A	317	-14.811	9.786	-31.076	1.00	14.83	A
ATOM	2471	C	ILE	A	317	-12.334	13.179	-29.487	1.00	14.51	A
ATOM	2472	O	ILE	A	317	-11.106	13.015	-29.353	1.00	13.70	A
ATOM	2473	N	GLY	A	318	-13.151	13.355	-28.452	1.00	11.91	A
ATOM	2474	CA	GLY	A	318	-12.635	13.353	-27.095	1.00	12.78	A
ATOM	2475	C	GLY	A	318	-12.935	12.063	-26.344	1.00	11.89	A
ATOM	2476	O	GLY	A	318	-13.880	11.343	-26.682	1.00	13.28	A
ATOM	2477	N	PHE	A	319	-12.125	11.754	-25.347	1.00	11.46	A
ATOM	2478	CA	PHE	A	319	-12.299	10.573	-24.517	1.00	13.15	A
ATOM	2479	CB	PHE	A	319	-11.423	9.386	-25.007	1.00	12.94	A
ATOM	2480	CG	PHE	A	319	-11.886	8.802	-26.316	1.00	15.51	A
ATOM	2481	CD1	PHE	A	319	-11.104	8.922	-27.448	1.00	17.96	A
ATOM	2482	CD2	PHE	A	319	-13.145	8.191	-26.426	1.00	16.52	A
ATOM	2483	CE1	PHE	A	319	-11.557	8.453	-28.684	1.00	16.81	A
ATOM	2484	CE2	PHE	A	319	-13.594	7.718	-27.660	1.00	17.65	A
ATOM	2485	CZ	PHE	A	319	-12.784	7.858	-28.794	1.00	20.90	A
ATOM	2486	O	PHE	A	319	-11.891	10.818	-23.103	1.00	12.47	A
ATOM	2487	C	PHE	A	319	-10.995	11.607	-22.820	1.00	12.56	A
ATOM	2488	N	ASN	A	320	-12.540	10.070	-22.217	1.00	12.28	A
ATOM	2489	CA	ASN	A	320	-12.241	10.066	-20.818	1.00	12.72	A
ATOM	2490	CB	ASN	A	320	-13.337	9.290	-20.074	1.00	15.27	A
ATOM	2491	CG	ASN	A	320	-13.046	9.141	-18.604	1.00	15.22	A
ATOM	2492	OD1	ASN	A	320	-12.276	8.268	-18.171	1.00	17.44	A
ATOM	2493	ND2	ASN	A	320	-13.668	9.997	-17.806	1.00	18.20	A
ATOM	2494	C	ASN	A	320	-10.919	9.318	-20.736	1.00	13.50	A
ATOM	2495	O	ASN	A	320	-10.775	8.232	-21.314	1.00	14.56	A
ATOM	2496	N	VAL	A	321	-9.948	9.923	-20.051	1.00	13.54	A
ATOM	2497	CA	VAL	A	321	-8.627	9.283	-19.905	1.00	15.24	A
ATOM	2498	CB	VAL	A	321	-7.661	10.211	-19.117	1.00	14.76	A
ATOM	2499	CG1	VAL	A	321	-6.363	9.465	-18.756	1.00	15.84	A
ATOM	2500	CG2	VAL	A	321	-7.370	11.417	-19.929	1.00	15.30	A
ATOM	2501	C	VAL	A	321	-8.620	7.936	-19.231	1.00	14.40	A
ATOM	2502	O	VAL	A	321	-8.011	6.999	-19.749	1.00	16.49	A
ATOM	2503	N	SER	A	322	-9.279	7.825	-18.093	1.00	14.64	A
ATOM	2504	CA	SER	A	322	-9.247	6.562	-17.370	1.00	16.47	A
ATOM	2505	CB	SER	A	322	-9.934	6.699	-15.995	1.00	18.37	A
ATOM	2506	CG	SER	A	322	-11.351	6.726	-16.106	1.00	22.86	A
ATOM	2507	C	SER	A	322	-9.852	5.443	-18.196	1.00	15.99	A
ATOM	2508	O	SER	A	322	-9.372	4.306	-18.142	1.00	14.69	A
ATOM	2509	N	TYR	A	323	-10.887	5.743	-18.986	1.00	15.32	A
ATOM	2510	CA	TYR	A	323	-11.497	4.659	-19.767	1.00	14.14	A
ATOM	2511	CB	TYR	A	323	-12.762	5.104	-20.509	1.00	13.38	A
ATOM	2512	CG	TYR	A	323	-13.911	5.510	-19.615	1.00	13.92	A
ATOM	2513	CD1	TYR	A	323	-13.925	5.195	-18.261	1.00	15.72	A
ATOM	2514	CE1	TYR	A	323	-15.014	5.562	-17.426	1.00	18.29	A
ATOM	2515	CE2	TYR	A	323	-14.992	6.184	-20.154	1.00	16.28	A
ATOM	2516	CZ	TYR	A	323	-16.080	6.546	-19.337	1.00	16.03	A
ATOM	2517	O	TYR	A	323	-16.074	6.238	-17.996	1.00	18.77	A
ATOM	2518	OH	TYR	A	323	-17.159	6.615	-17.192	1.00	19.53	A
ATOM	2519	C	TYR	A	323	-10.522	4.097	-20.798	1.00	13.72	A
ATOM	2520	O	TYR	A	323	-10.472	2.871	-20.988	1.00	14.43	A
ATOM	2521	N	VAL	A	324	-9.766	4.979	-21.458	1.00	14.57	A
ATOM	2522	CA	VAL	A	324	-8.827	4.508	-22.469	1.00	13.06	A
ATOM	2523	CB	VAL	A	324	-8.372	5.662	-23.389	1.00	13.33	A
ATOM	2524	CG1	VAL	A	324	-7.307	5.165	-24.365	1.00	13.38	A
ATOM	2525	CG2	VAL	A	324	-9.556	6.227	-24.142	1.00	13.06	A
ATOM	2526	C	VAL	A	324	-7.625	3.863	-21.805	1.00	13.51	A
ATOM	2527	O	VAL	A	324	-7.180	2.778	-22.239	1.00	13.91	A
ATOM	2528	N	LEU	A	325	-7.103	4.485	-20.749	1.00	13.19	A
ATOM	2529	CA	LEU	A	325	-5.958	3.856	-20.062	1.00	12.30	A
ATOM	2530	CB	LEU	A	325	-5.421	4.740	-18.922	1.00	14.09	A
ATOM	2531	CG	LEU	A	325	-4.756	6.018	-19.451	1.00	15.74	A
ATOM	2532	CD1	LEU	A	325	-4.309	6.898	-18.293	1.00	16.69	A
ATOM	2533	CD2	LEU	A	325	-3.511	5.670	-20.297	1.00	16.07	A
ATOM	2534	C	LEU	A	325	-6.340	2.486	-19.523	1.00	12.94	A
ATOM	2535	O	LEU	A	325	-5.530	1.561	-19.557	1.00	13.40	A
ATOM	2536	N	ASP	A	326	-7.558	2.333	-18.993	1.00	12.70	A
ATOM	2537	CA	ASP	A	326	-7.979	1.036	-18.483	1.00	13.88	A
ATOM	2538	CB	ASP	A	326	-9.424	1.066	-17.982	1.00	15.00	A
ATOM	2539	CG	ASP	A	326	-9.580	1.726	-16.613	1.00	18.64	A
ATOM	2540	OD1	ASP	A	326	-8.568	1.979	-15.900	1.00	17.79	A
ATOM	2541	OD2	ASP	A	326	-10.754	2.016	-16.228	1.00	17.43	A
ATOM	2542	C	ASP	A	326	-7.882	-0.010	-19.589	1.00	11.78	A
ATOM	2543	O	ASP	A	326	-7.433	-1.134	-19.355	1.00	14.48	A
ATOM	2544	N	VAL	A	327	-8.349	0.350	-20.785	1.00	12.78	A
ATOM	2545	CA	VAL	A	327	-8.317	-0.577	-21.919	1.00	12.19	A
ATOM	2546	CB	VAL	A	327	-9.036	0.029	-23.136	1.00	13.17	A
ATOM	2547	CG1	VAL	A	327	-8.820	-0.794	-24.388	1.00	13.91	A
ATOM	2548	CG2	VAL	A	327	-10.544	0.097	-22.800	1.00	11.68	A
ATOM	2549	C	VAL	A	327	-6.889	-0.925	-22.325	1.00	12.85	A
ATOM	2550	O	VAL	A	327	-6.582	-2.089	-22.542	1.00	13.03	A
ATOM	2551	N	LEU	A	328	-6.037	0.086	-22.418	1.00	13.64	A
ATOM	2552	CA	LEU	A	328	-4.646	-0.142	-22.856	1.00	13.56	A
ATOM	2553	CB	LEU	A	328	-3.949	1.201	-23.100	1.00	12.03	A
ATOM	2554	CG	LEU	A	328	-4.626	2.058	-24.192	1.00	13.75	A
ATOM	2555	CD1	LEU	A	328	-3.799	3.306	-24.432	1.00	14.51	A
ATOM	2556	CD2	LEU	A	328	-4.758	1.252	-25.503	1.00	15.65	A
ATOM	2557	C	LEU	A	328	-3.888	-0.972	-21.825	1.00	16.00	A
ATOM	2558	O	LEU	A	328	-2.982	-1.748	-22.174	1.00	17.28	A
ATOM	2559	N	ASN	A	329	-4.252	-0.830	-20.557	1.00	14.82	A
ATOM	2560	CA	ASN	A	329	-3.639	-1.609	-19.486	1.00	16.78	A
ATOM	2561	CB	ASN	A	329	-3.965	-0.957	-18.143	1.00	18.81	A
ATOM	2562	CG	ASN	A	329	-3.039	0.182	-17.815	1.00	22.88	A
ATOM	2563	OD1	ASN	A	329	-3.410	1.088	-17.067	1.00	27.05	A
ATOM	2564	ND2	ASN	A	329	-1.810	0.139	-18.340	1.00	24.22	A
ATOM	2565	C	ASN	A	329	-4.112	-3.059	-19.522	1.00	19.68	A

Figure 1 (continued 26)

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ATOM	2566	O	ASN	A	329	-3.353	-3.984	-19.177	1.00	20.96	A
ATOM	2567	N	ALA	A	330	-5.347	-3.282	-19.966	1.00	18.19	A
ATOM	2568	CA	ALA	A	330	-5.893	-4.635	-20.059	1.00	20.30	A
ATOM	2569	CB	ALA	A	330	-7.444	-4.597	-20.070	1.00	20.07	A
ATOM	2570	C	ALA	A	330	-5.385	-5.363	-21.304	1.00	20.84	A
ATOM	2571	O	ALA	A	330	-5.261	-6.601	-21.302	1.00	21.96	A
ATOM	2572	N	LEU	A	331	-5.092	-4.614	-22.365	1.00	20.51	A
ATOM	2573	CA	LEU	A	331	-4.607	-5.238	-23.606	1.00	22.56	A
ATOM	2574	CB	LEU	A	331	-4.857	-4.311	-24.807	1.00	19.58	A
ATOM	2575	CG	LEU	A	331	-6.319	-4.242	-25.284	1.00	20.93	A
ATOM	2576	CD1	LEU	A	331	-6.493	-3.076	-26.290	1.00	20.46	A
ATOM	2577	CD2	LEU	A	331	-6.749	-5.570	-25.905	1.00	19.08	A
ATOM	2578	C	LEU	A	331	-3.127	-5.621	-23.508	1.00	25.46	A
ATOM	2579	O	LEU	A	331	-2.742	-6.688	-23.998	1.00	27.06	A
ATOM	2580	N	LYS	A	332	-2.313	-4.753	-22.903	1.00	26.68	A
ATOM	2581	CA	LYS	A	332	-0.877	-5.002	-22.724	1.00	28.23	A
ATOM	2582	CB	LYS	A	332	-0.651	-5.661	-21.356	1.00	29.27	A
ATOM	2583	CG	LYS	A	332	-1.401	-6.966	-21.184	1.00	29.90	A
ATOM	2584	CD	LYS	A	332	-1.468	-7.412	-19.728	1.00	32.09	A
ATOM	2585	CE	LYS	A	332	-2.173	-8.745	-19.658	1.00	32.35	A
ATOM	2586	NZ	LYS	A	332	-2.345	-9.225	-18.268	1.00	35.40	A
ATOM	2587	C	LYS	A	332	-0.266	-5.853	-23.855	1.00	27.53	A
ATOM	2588	O	LYS	A	332	0.361	-6.884	-23.618	1.00	31.18	A
ATOM	2589	N	CYS	A	333	-0.484	-5.404	-25.087	1.00	25.22	A
ATOM	2590	CA	CYS	A	333	0.010	-6.074	-26.301	1.00	21.25	A
ATOM	2591	CB	CYS	A	333	-1.158	-6.522	-27.166	1.00	19.35	A
ATOM	2592	SG	CYS	A	333	-2.257	-5.131	-27.559	1.00	20.24	A
ATOM	2593	C	CYS	A	333	0.878	-5.087	-27.069	1.00	20.62	A
ATOM	2594	O	CYS	A	333	1.047	-3.966	-26.640	1.00	20.60	A
ATOM	2595	N	GLU	A	334	1.422	-5.490	-28.218	1.00	19.42	A
ATOM	2596	CA	GLU	A	334	2.317	-4.604	-28.956	1.00	19.82	A
ATOM	2597	CB	GLU	A	334	3.102	-5.421	-29.998	1.00	21.89	A
ATOM	2598	CG	GLU	A	334	4.169	-4.662	-30.765	1.00	27.12	A
ATOM	2599	CD	GLU	A	334	5.320	-4.181	-29.882	1.00	29.45	A
ATOM	2600	OE1	GLU	A	334	5.657	-4.863	-28.890	1.00	32.60	A
ATOM	2601	OE2	GLU	A	334	5.902	-3.121	-30.198	1.00	32.88	A
ATOM	2602	C	GLU	A	334	1.625	-3.429	-29.636	1.00	16.58	A
ATOM	2603	O	GLU	A	334	2.060	-2.292	-29.474	1.00	16.78	A
ATOM	2604	N	ASN	A	335	0.576	-3.704	-30.402	1.00	16.51	A
ATOM	2605	CA	ASN	A	335	-0.146	-2.651	-31.136	1.00	15.36	A
ATOM	2606	CB	ASN	A	335	0.089	-2.780	-32.646	1.00	18.00	A
ATOM	2607	CG	ASN	A	335	1.546	-2.690	-33.022	1.00	20.47	A
ATOM	2608	OD1	ASN	A	335	2.162	-3.672	-33.464	1.00	25.38	A
ATOM	2609	ND2	ASN	A	335	2.103	-1.518	-32.867	1.00	18.14	A
ATOM	2610	C	ASN	A	335	-1.646	-2.792	-30.914	1.00	16.50	A
ATOM	2611	O	ASN	A	335	-2.167	-3.914	-30.726	1.00	16.59	A
ATOM	2612	N	VAL	A	336	-2.327	-1.661	-30.918	1.00	16.20	A
ATOM	2613	CA	VAL	A	336	-3.764	-1.655	-30.767	1.00	14.76	A
ATOM	2614	CB	VAL	A	336	-4.247	-0.853	-29.501	1.00	16.01	A
ATOM	2615	CG1	VAL	A	336	-3.681	-1.469	-28.239	1.00	19.32	A
ATOM	2616	CG2	VAL	A	336	-3.854	0.619	-29.614	1.00	18.64	A
ATOM	2617	C	VAL	A	336	-4.390	-1.040	-31.993	1.00	16.20	A
ATOM	2618	O	VAL	A	336	-3.766	-0.257	-32.719	1.00	15.92	A
ATOM	2619	N	ARG	A	337	-5.631	-1.422	-32.238	1.00	16.08	A
ATOM	2620	CA	ARG	A	337	-6.391	-0.860	-33.330	1.00	17.59	A
ATOM	2621	CB	ARG	A	337	-6.879	-1.961	-34.281	1.00	20.37	A
ATOM	2622	CG	ARG	A	337	-7.779	-1.445	-35.423	1.00	24.09	A
ATOM	2623	CD	ARG	A	337	-8.161	-2.499	-36.481	1.00	26.96	A
ATOM	2624	NE	ARG	A	337	-6.983	-3.165	-37.020	1.00	29.58	A
ATOM	2625	CZ	ARG	A	337	-6.568	-4.265	-36.628	1.00	30.93	A
ATOM	2626	NH1	ARG	A	337	-7.254	-5.040	-35.706	1.00	33.27	A
ATOM	2627	NH2	ARG	A	337	-5.446	-4.880	-37.124	1.00	31.58	A
ATOM	2628	C	ARG	A	337	-7.602	-0.160	-32.741	1.00	17.83	A
ATOM	2629	O	ARG	A	337	-8.342	-0.739	-31.919	1.00	17.99	A
ATOM	2630	N	MET	A	338	-7.803	1.092	-33.154	1.00	16.35	A
ATOM	2631	CA	MET	A	338	-8.976	1.881	-32.731	1.00	17.54	A
ATOM	2632	CB	MET	A	338	-8.561	3.298	-32.322	1.00	19.03	A
ATOM	2633	CG	MET	A	338	-7.696	3.343	-31.067	1.00	22.98	A
ATOM	2634	SD	MET	A	338	-7.251	5.013	-30.485	1.00	28.14	A
ATOM	2635	CE	MET	A	338	-8.672	5.347	-29.411	1.00	24.78	A
ATOM	2636	C	MET	A	338	-9.867	1.943	-33.963	1.00	17.28	A
ATOM	2637	O	MET	A	338	-9.398	2.321	-35.063	1.00	18.78	A
ATOM	2638	N	MET	A	339	-11.144	1.591	-33.825	1.00	17.39	A
ATOM	2639	CA	MET	A	339	-12.064	1.582	-34.955	1.00	17.39	A
ATOM	2640	CB	MET	A	339	-12.686	0.180	-35.053	1.00	20.98	A
ATOM	2641	CG	MET	A	339	-11.628	-0.888	-34.852	1.00	25.07	A
ATOM	2642	SD	MET	A	339	-12.307	-2.536	-34.442	1.00	30.90	A
ATOM	2643	CE	MET	A	339	-12.758	-2.891	-36.141	1.00	27.62	A
ATOM	2644	C	MET	A	339	-13.075	2.676	-34.673	1.00	18.45	A
ATOM	2645	O	MET	A	339	-13.868	2.596	-33.729	1.00	17.17	A
ATOM	2646	N	LEU	A	340	-13.009	3.728	-35.490	1.00	17.41	A
ATOM	2647	CA	LEU	A	340	-13.853	4.898	-35.313	1.00	19.07	A
ATOM	2648	CB	LEU	A	340	-12.974	6.150	-35.330	1.00	21.15	A
ATOM	2649	CG	LEU	A	340	-11.856	6.140	-34.291	1.00	22.56	A
ATOM	2650	CD1	LEU	A	340	-10.597	6.765	-34.885	1.00	27.71	A
ATOM	2651	CD2	LEU	A	340	-12.321	6.886	-33.043	1.00	24.99	A
ATOM	2652	C	LEU	A	340	-14.892	5.036	-36.396	1.00	20.06	A
ATOM	2653	O	LEU	A	340	-14.739	4.483	-37.481	1.00	20.26	A
ATOM	2654	N	THR	A	341	-15.941	5.783	-36.086	1.00	22.17	A
ATOM	2655	CA	THR	A	341	-17.029	6.020	-37.026	1.00	25.08	A
ATOM	2656	CB	THR	A	341	-18.360	5.576	-36.433	1.00	26.10	A
ATOM	2657	OG1	THR	A	341	-18.287	4.178	-36.133	1.00	25.61	A
ATOM	2658	CG2	THR	A	341	-19.487	5.811	-37.438	1.00	26.42	A
ATOM	2659	C	THR	A	341	-17.084	7.509	-37.328	1.00	25.45	A
ATOM	2660	O	THR	A	341	-16.921	7.922	-38.481	1.00	27.99	A
ATOM	2661	N	ASP	A	342	-17.320	8.298	-36.284	1.00	25.19	A
ATOM	2662	CA	ASP	A	342	-17.367	9.757	-36.381	1.00	24.72	A
ATOM	2663	CB	ASP	A	342	-18.690	10.235	-37.008	1.00	25.68	A
ATOM	2664	CG	ASP	A	342	-19.905	9.816	-36.214	1.00	27.08	A
ATOM	2665	OD1	ASP	A	342	-19.828	9.819	-34.967	1.00	25.89	A

Figure 1 (continued 27)

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ATOM	2666	OD2	ASP	A	342	-20.947	9.513	-36.855	1.00	30.26	A
ATOM	2667	C	ASP	A	342	-17.137	10.406	-35.019	1.00	23.68	A
ATOM	2668	O	ASP	A	342	-16.889	9.725	-34.014	1.00	21.46	A
ATOM	2669	N	SER	A	343	-17.216	11.729	-34.969	1.00	23.14	A
ATOM	2670	C	SER	A	343	-16.929	12.436	-33.744	1.00	24.43	A
ATOM	2671	CB	SER	A	343	-16.755	13.936	-34.034	1.00	26.47	A
ATOM	2672	OG	SER	A	343	-17.994	14.549	-34.368	1.00	29.79	A
ATOM	2673	C	SER	A	343	-17.905	12.249	-32.602	1.00	24.03	A
ATOM	2674	O	SER	A	343	-17.567	12.520	-31.457	1.00	24.30	A
ATOM	2675	N	VAL	A	344	-19.109	11.758	-32.884	1.00	23.83	A
ATOM	2676	CA	VAL	A	344	-20.078	11.630	-31.809	1.00	23.12	A
ATOM	2677	CB	VAL	A	344	-21.357	12.448	-32.132	1.00	24.91	A
ATOM	2678	CG1	VAL	A	344	-21.003	13.909	-32.356	1.00	25.01	A
ATOM	2679	CG2	VAL	A	344	-22.011	11.888	-33.359	1.00	23.59	A
ATOM	2680	C	VAL	A	344	-20.487	10.192	-31.504	1.00	23.42	A
ATOM	2681	O	VAL	A	344	-21.458	9.951	-30.788	1.00	25.49	A
ATOM	2682	N	SER	A	345	-19.731	9.244	-32.026	1.00	21.89	A
ATOM	2683	CA	SER	A	345	-20.013	7.829	-31.834	1.00	21.04	A
ATOM	2684	CB	SER	A	345	-20.163	7.177	-33.197	1.00	22.41	A
ATOM	2685	OG	SER	A	345	-21.229	7.826	-33.898	1.00	25.59	A
ATOM	2686	C	SER	A	345	-18.903	7.139	-31.038	1.00	20.75	A
ATOM	2687	O	SER	A	345	-17.768	7.582	-31.036	1.00	20.76	A
ATOM	2688	N	SER	A	346	-19.241	6.045	-30.367	1.00	18.72	A
ATOM	2689	CA	SER	A	346	-18.246	5.325	-29.580	1.00	17.41	A
ATOM	2690	CB	SER	A	346	-18.942	4.243	-28.764	1.00	18.74	A
ATOM	2691	O	SER	A	346	-19.913	4.838	-27.930	1.00	22.66	A
ATOM	2692	C	SER	A	346	-17.184	4.697	-30.466	1.00	17.40	A
ATOM	2693	O	SER	A	346	-17.398	4.490	-31.656	1.00	21.59	A
ATOM	2694	N	VAL	A	347	-16.045	4.390	-29.869	1.00	16.03	A
ATOM	2695	CA	VAL	A	347	-14.916	3.754	-30.558	1.00	15.59	A
ATOM	2696	CB	VAL	A	347	-13.561	4.492	-30.225	1.00	16.49	A
ATOM	2697	CG1	VAL	A	347	-13.206	4.415	-28.731	1.00	17.48	A
ATOM	2698	CG2	VAL	A	347	-12.426	3.924	-31.045	1.00	19.46	A
ATOM	2699	C	VAL	A	347	-14.809	2.305	-30.088	1.00	14.00	A
ATOM	2700	O	VAL	A	347	-15.213	2.005	-28.974	1.00	15.79	A
ATOM	2701	N	GLN	A	348	-14.340	1.420	-30.957	1.00	13.62	A
ATOM	2702	CA	GLN	A	348	-14.081	0.025	-30.547	1.00	12.23	A
ATOM	2703	CB	GLN	A	348	-14.702	-0.983	-31.533	1.00	13.64	A
ATOM	2704	CG	GLN	A	348	-14.416	-2.454	-31.162	1.00	15.65	A
ATOM	2705	CD	GLN	A	348	-15.268	-3.431	-31.957	1.00	16.97	A
ATOM	2706	OE1	GLN	A	348	-14.825	-4.545	-32.272	1.00	22.42	A
ATOM	2707	NE2	GLN	A	348	-16.499	-3.035	-32.262	1.00	16.85	A
ATOM	2708	C	GLN	A	348	-12.548	-0.121	-30.580	1.00	13.90	A
ATOM	2709	O	GLN	A	348	-11.909	0.275	-31.563	1.00	13.82	A
ATOM	2710	N	ILE	A	349	-11.971	-0.681	-29.513	1.00	12.76	A
ATOM	2711	CA	ILE	A	349	-10.516	-0.865	-29.425	1.00	12.30	A
ATOM	2712	CB	ILE	A	349	-9.967	-0.071	-28.210	1.00	14.15	A
ATOM	2713	CG2	ILE	A	349	-8.434	-0.148	-28.138	1.00	14.43	A
ATOM	2714	CG1	ILE	A	349	-10.359	1.398	-28.357	1.00	13.90	A
ATOM	2715	CD1	ILE	A	349	-9.959	2.196	-27.088	1.00	14.25	A
ATOM	2716	C	ILE	A	349	-10.232	-2.339	-29.247	1.00	14.06	A
ATOM	2717	O	ILE	A	349	-10.933	-3.012	-28.480	1.00	14.91	A
ATOM	2718	N	GLU	A	350	-9.195	-2.824	-29.938	1.00	14.83	A
ATOM	2719	CA	GLU	A	350	-8.765	-4.231	-29.850	1.00	15.53	A
ATOM	2720	CB	GLU	A	350	-9.357	-5.077	-30.975	1.00	17.90	A
ATOM	2721	CG	GLU	A	350	-10.870	-5.018	-31.138	1.00	19.30	A
ATOM	2722	CD	GLU	A	350	-11.361	-5.919	-32.260	1.00	24.15	A
ATOM	2723	OE1	GLU	A	350	-10.523	-6.447	-33.034	1.00	25.09	A
ATOM	2724	OE2	GLU	A	350	-12.589	-6.095	-32.374	1.00	23.78	A
ATOM	2725	C	GLU	A	350	-7.247	-4.312	-30.037	1.00	15.60	A
ATOM	2726	O	GLU	A	350	-6.600	-3.359	-30.479	1.00	15.29	A
ATOM	2727	N	ASP	A	351	-6.693	-5.471	-29.693	1.00	16.12	A
ATOM	2728	CA	ASP	A	351	-5.276	-5.765	-29.898	1.00	15.76	A
ATOM	2729	CB	ASP	A	351	-4.976	-7.144	-29.283	1.00	15.10	A
ATOM	2730	CG	ASP	A	351	-3.542	-7.604	-29.489	1.00	17.20	A
ATOM	2731	OD1	ASP	A	351	-2.865	-7.057	-30.377	1.00	17.43	A
ATOM	2732	OD2	ASP	A	351	-3.085	-8.526	-28.744	1.00	18.87	A
ATOM	2733	C	ASP	A	351	-5.253	-5.849	-31.438	1.00	15.75	A
ATOM	2734	O	ASP	A	351	-6.140	-6.458	-32.049	1.00	16.51	A
ATOM	2735	N	ALA	A	352	-4.278	-5.224	-32.096	1.00	16.21	A
ATOM	2736	CA	ALA	A	352	-4.269	-5.276	-33.558	1.00	18.09	A
ATOM	2737	CB	ALA	A	352	-3.158	-4.347	-34.121	1.00	18.36	A
ATOM	2738	CG	ALA	A	352	-4.046	-6.711	-34.030	1.00	18.81	A
ATOM	2739	CD	ALA	A	352	-4.396	-7.044	-35.158	1.00	21.06	A
ATOM	2740	OE1	ALA	A	353	-3.496	-7.552	-33.157	1.00	19.56	A
ATOM	2741	OE2	ALA	A	353	-3.194	-8.946	-33.502	1.00	20.21	A
ATOM	2742	C	ALA	A	353	-1.792	-9.285	-33.026	1.00	20.26	A
ATOM	2743	O	ALA	A	353	-4.167	-10.006	-32.977	1.00	21.68	A
ATOM	2744	N	ALA	A	353	-3.901	-11.201	-33.108	1.00	23.17	A
ATOM	2745	CA	SER	A	354	-5.281	-9.598	-32.382	1.00	20.83	A
ATOM	2746	CB	SER	A	354	-6.225	-10.577	-31.843	1.00	19.77	A
ATOM	2747	CG	SER	A	354	-5.780	-11.029	-30.468	1.00	20.42	A
ATOM	2748	OG	SER	A	354	-6.738	-11.943	-29.917	1.00	22.32	A
ATOM	2749	C	SER	A	354	-7.597	-9.986	-31.687	1.00	20.59	A
ATOM	2750	O	SER	A	354	-7.720	-8.890	-31.151	1.00	19.79	A
ATOM	2751	N	GLN	A	355	-8.618	-10.720	-32.129	1.00	20.97	A
ATOM	2752	CA	GLN	A	355	-9.990	-10.266	-32.014	1.00	22.47	A
ATOM	2753	CB	GLN	A	355	-10.786	-10.602	-33.278	1.00	26.42	A
ATOM	2754	CG	GLN	A	355	-10.487	-9.680	-34.457	1.00	29.56	A
ATOM	2755	CD	GLN	A	355	-11.532	-9.777	-35.552	1.00	32.83	A
ATOM	2756	OE1	GLN	A	355	-12.725	-9.567	-35.307	1.00	34.38	A
ATOM	2757	NE2	GLN	A	355	-11.088	-10.083	-36.773	1.00	33.96	A
ATOM	2758	C	GLN	A	355	-10.664	-10.924	-30.809	1.00	20.74	A
ATOM	2759	O	GLN	A	355	-11.869	-10.815	-30.648	1.00	23.27	A
ATOM	2760	N	SER	A	356	-9.887	-11.573	-29.956	1.00	18.84	A
ATOM	2761	CA	SER	A	356	-10.456	-12.239	-28.769	1.00	19.15	A
ATOM	2762	CB	SER	A	356	-9.386	-13.050	-28.027	1.00	19.93	A
ATOM	2763	OG	SER	A	356	-8.338	-12.230	-27.573	1.00	26.23	A
ATOM	2764	C	SER	A	356	-11.136	-11.293	-27.793	1.00	17.16	A
ATOM	2765	O	SER	A	356	-12.118	-11.664	-27.158	1.00	17.71	A

Figure 1 (continued 28)

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ATOM	2766	N	ALA	A	357	-10.623	-10.084	-27.649	1.00	16.33	A
ATOM	2767	CA	ALA	A	357	-11.258	-9.113	-26.750	1.00	16.01	A
ATOM	2768	CB	ALA	A	357	-10.362	-8.779	-25.603	1.00	17.39	A
ATOM	2769	C	ALA	A	357	-11.590	-7.841	-27.524	1.00	15.77	A
ATOM	2770	O	ALA	A	357	-10.883	-7.481	-28.477	1.00	18.23	A
ATOM	2771	N	ALA	A	358	-12.673	-7.180	-27.129	1.00	15.41	A
ATOM	2772	CA	ALA	A	358	-13.047	-5.907	-27.761	1.00	12.42	A
ATOM	2773	CB	ALA	A	358	-14.140	-6.118	-28.811	1.00	14.36	A
ATOM	2774	C	ALA	A	358	-13.535	-4.944	-26.677	1.00	13.39	A
ATOM	2775	O	ALA	A	358	-14.168	-5.354	-25.689	1.00	13.08	A
ATOM	2776	N	TYR	A	359	-13.250	-3.662	-26.853	1.00	11.92	A
ATOM	2777	CA	TYR	A	359	-13.638	-2.664	-25.873	1.00	12.31	A
ATOM	2778	CB	TYR	A	359	-12.385	-2.123	-25.143	1.00	12.39	A
ATOM	2779	CG	TYR	A	359	-11.605	-3.220	-24.463	1.00	12.04	A
ATOM	2780	CD1	TYR	A	359	-11.895	-3.596	-23.151	1.00	11.11	A
ATOM	2781	CE1	TYR	A	359	-11.257	-4.683	-22.558	1.00	12.06	A
ATOM	2782	CD2	TYR	A	359	-10.643	-3.958	-25.175	1.00	12.43	A
ATOM	2783	CE2	TYR	A	359	-10.014	-5.054	-24.588	1.00	12.80	A
ATOM	2784	CZ	TYR	A	359	-10.328	-5.396	-23.286	1.00	13.52	A
ATOM	2785	OH	TYR	A	359	-9.685	-6.468	-22.703	1.00	14.61	A
ATOM	2786	C	TYR	A	359	-14.380	-1.543	-26.564	1.00	12.62	A
ATOM	2787	O	TYR	A	359	-14.014	-1.160	-27.671	1.00	13.90	A
ATOM	2788	N	VAL	A	360	-15.470	-1.072	-25.961	1.00	12.93	A
ATOM	2789	CA	VAL	A	360	-16.245	0.015	-26.567	1.00	14.00	A
ATOM	2790	CB	VAL	A	360	-17.670	-0.433	-26.861	1.00	12.46	A
ATOM	2791	CG1	VAL	A	360	-18.476	0.737	-27.477	1.00	15.11	A
ATOM	2792	CG2	VAL	A	360	-17.624	-1.638	-27.791	1.00	14.89	A
ATOM	2793	C	VAL	A	360	-16.255	1.158	-25.586	1.00	13.57	A
ATOM	2794	O	VAL	A	360	-16.573	0.967	-24.419	1.00	12.80	A
ATOM	2795	N	VAL	A	361	-15.883	2.359	-26.044	1.00	13.11	A
ATOM	2796	CA	VAL	A	361	-15.821	3.496	-25.157	1.00	14.02	A
ATOM	2797	CB	VAL	A	361	-14.346	3.931	-24.924	1.00	13.31	A
ATOM	2798	CG1	VAL	A	361	-14.272	5.047	-23.911	1.00	14.14	A
ATOM	2799	CG2	VAL	A	361	-13.542	2.718	-24.402	1.00	13.41	A
ATOM	2800	C	VAL	A	361	-16.566	4.648	-25.785	1.00	13.82	A
ATOM	2801	O	VAL	A	361	-16.339	4.947	-26.948	1.00	14.34	A
ATOM	2802	N	MET	A	362	-17.494	5.247	-25.043	1.00	15.43	A
ATOM	2803	CA	MET	A	362	-18.208	6.383	-25.612	1.00	17.04	A
ATOM	2804	CB	MET	A	362	-19.406	6.802	-24.729	1.00	24.10	A
ATOM	2805	CG	MET	A	362	-20.532	5.811	-24.542	1.00	30.22	A
ATOM	2806	SD	MET	A	362	-21.744	6.650	-22.450	1.00	27.70	A
ATOM	2807	CE	MET	A	362	-20.595	7.445	-22.182	1.00	16.05	A
ATOM	2808	C	MET	A	362	-17.290	7.592	-25.674	1.00	16.00	A
ATOM	2809	O	MET	A	362	-16.327	7.689	-24.949	1.00	16.34	A
ATOM	2810	N	PRO	A	363	-17.602	8.535	-26.550	1.00	19.07	A
ATOM	2811	CD	PRO	A	363	-18.565	8.438	-27.661	1.00	17.39	A
ATOM	2812	CA	PRO	A	363	-16.771	9.736	-26.643	1.00	20.19	A
ATOM	2813	CB	PRO	A	363	-17.127	10.292	-28.017	1.00	20.14	A
ATOM	2814	CG	PRO	A	363	-18.547	9.841	-28.237	1.00	18.96	A
ATOM	2815	PRO	PRO	A	363	-17.113	10.686	-25.490	1.00	19.41	A
ATOM	2816	O	PRO	A	364	-18.201	10.583	-24.888	1.00	17.22	A
ATOM	2817	C	PRO	A	364	-16.172	11.557	-25.138	1.00	16.88	A
ATOM	2818	N	MET	A	364	-16.369	12.584	-24.095	1.00	18.63	A
ATOM	2819	CA	MET	A	364	-15.308	12.451	-22.998	1.00	19.86	A
ATOM	2820	CB	MET	A	364	-15.448	13.444	-21.856	1.00	20.18	A
ATOM	2821	SD	MET	A	364	-14.143	13.161	-20.684	1.00	21.47	A
ATOM	2822	CE	MET	A	364	-14.902	12.079	-19.580	1.00	19.03	A
ATOM	2823	C	MET	A	364	-16.309	13.976	-24.722	1.00	19.46	A
ATOM	2824	O	MET	A	364	-15.394	14.297	-25.489	1.00	18.40	A
ATOM	2825	N	ARG	A	365	-17.297	14.828	-24.430	1.00	21.57	A
ATOM	2826	CA	ARG	A	365	-17.304	16.180	-24.984	1.00	23.93	A
ATOM	2827	CB	ARG	A	365	-18.723	16.759	-24.976	1.00	30.14	A
ATOM	2828	CG	ARG	A	365	-19.660	16.122	-25.961	1.00	35.93	A
ATOM	2829	CD	ARG	A	365	-19.240	16.437	-27.376	1.00	41.53	A
ATOM	2830	NE	ARG	A	365	-20.353	16.314	-28.317	1.00	43.21	A
ATOM	2831	CZ	ARG	A	365	-20.214	16.365	-29.639	1.00	43.54	A
ATOM	2832	NH1	ARG	A	365	-19.009	16.526	-30.174	1.00	44.53	A
ATOM	2833	NH2	ARG	A	365	-21.281	16.282	-30.426	1.00	20.31	A
ATOM	2834	C	ARG	A	365	-16.402	17.079	-24.164	1.00	19.99	A
ATOM	2835	O	ARG	A	365	-16.487	17.099	-22.932	1.00	19.74	A
ATOM	2836	N	LEU	A	366	-15.549	17.842	-24.850	1.00	21.42	A
ATOM	2837	CA	LEU	A	366	-14.637	18.744	-24.152	1.00	21.30	A
ATOM	2838	CB	LEU	A	366	-13.205	18.186	-24.236	1.00	22.44	A
ATOM	2839	CG	LEU	A	366	-12.987	16.831	-23.568	1.00	22.25	A
ATOM	2840	CD1	LEU	A	366	-11.670	16.240	-24.049	1.00	21.14	A
ATOM	2841	CD2	LEU	A	366	-12.952	16.997	-22.073	1.00	23.50	A
ATOM	2842	C	LEU	A	366	-14.675	20.182	-24.703	1.00	24.15	A
ATOM	2843	O	LEU	A	366	-13.631	20.879	-24.600	1.00	25.87	A
ATOM	2844	OX	LEU	A	366	-15.757	20.610	-25.202	1.00	14.72	B
ATOM	2845	CE	MET	B	1	14.354	31.226	-16.722	1.00	13.54	B
ATOM	2846	CG	MET	B	1	14.917	30.008	-15.980	1.00	17.51	B
ATOM	2847	SD	MET	B	1	13.753	29.266	-14.804	1.00	16.34	B
ATOM	2848	CE	MET	B	1	12.697	28.387	-15.952	1.00	14.66	B
ATOM	2849	C	MET	B	1	14.966	30.414	-18.998	1.00	16.39	B
ATOM	2850	O	MET	B	1	13.867	30.217	-19.542	1.00	16.03	B
ATOM	2851	N	MET	B	1	14.668	32.827	-18.638	1.00	13.94	B
ATOM	2852	N	MET	B	1	15.135	31.538	-18.017	1.00	14.97	B
ATOM	2853	N	LYS	B	2	16.047	29.666	-19.238	1.00	15.37	B
ATOM	2854	CA	LYS	B	2	16.015	28.554	-20.195	1.00	17.84	B
ATOM	2855	CB	LYS	B	2	16.413	29.068	-21.575	1.00	23.16	B
ATOM	2856	CG	LYS	B	2	16.273	28.083	-22.709	1.00	27.33	B
ATOM	2857	CD	LYS	B	2	16.371	28.841	-24.054	1.00	30.66	B
ATOM	2858	CE	LYS	B	2	15.972	27.950	-25.222	1.00	31.91	B
ATOM	2859	CZ	LYS	B	2	16.920	26.805	-25.375	1.00	16.00	B
ATOM	2860	N	LYS	B	2	17.004	27.477	-19.805	1.00	14.43	B
ATOM	2861	O	LYS	B	2	18.106	27.776	-19.356	1.00	12.71	B
ATOM	2862	C	PHE	B	3	16.592	26.224	-19.918	1.00	13.78	B
ATOM	2863	CA	PHE	B	3	17.524	25.132	-19.669	1.00	12.36	B
ATOM	2864	CB	PHE	B	3	17.744	24.912	-18.154	1.00	11.46	B
ATOM	2865	CG	PHE	B	3	16.521	24.464	-17.403	1.00		B

Figure 1 (continued 29)

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ATOM	2866	CD1	PHE	B	3	15.726	25.391	-16.719	1.00	12.95	B
ATOM	2867	CD2	PHE	B	3	16.192	23.108	-17.354	1.00	11.17	B
ATOM	2868	CE1	PHE	B	3	14.607	24.944	-15.988	1.00	13.10	B
ATOM	2869	CE2	PHE	B	3	15.088	22.664	-16.639	1.00	13.73	B
ATOM	2870	CZ	PHE	B	3	14.300	23.594	-15.956	1.00	11.90	B
ATOM	2871	O	PHE	B	3	17.047	23.862	-20.358	1.00	12.91	B
ATOM	2872	O	PHE	B	3	15.870	23.705	-20.657	1.00	14.61	B
ATOM	2873	N	THR	B	4	17.981	22.983	-20.677	1.00	12.44	B
ATOM	2874	CA	THR	B	4	17.647	21.694	-21.264	1.00	12.80	B
ATOM	2875	CB	THR	B	4	18.054	21.570	-22.727	1.00	14.32	B
ATOM	2876	OG1	THR	B	4	17.465	22.636	-23.492	1.00	17.57	B
ATOM	2877	CG2	THR	B	4	17.564	20.235	-23.258	1.00	15.46	B
ATOM	2878	O	THR	B	4	18.437	20.668	-20.440	1.00	14.04	B
ATOM	2879	O	THR	B	4	19.658	20.774	-20.291	1.00	14.28	B
ATOM	2880	N	VAL	B	5	17.740	19.692	-19.870	1.00	14.07	B
ATOM	2881	CA	VAL	B	5	18.377	18.702	-19.003	1.00	14.50	B
ATOM	2882	CB	VAL	B	5	18.137	19.055	-17.497	1.00	14.63	B
ATOM	2883	CG1	VAL	B	5	18.774	17.995	-16.572	1.00	19.00	B
ATOM	2884	CG2	VAL	B	5	18.711	20.379	-17.153	1.00	19.65	B
ATOM	2885	O	VAL	B	5	17.841	17.296	-19.293	1.00	16.13	B
ATOM	2886	O	VAL	B	5	16.685	17.117	-19.675	1.00	16.46	B
ATOM	2887	N	GLU	B	6	18.694	16.294	-19.151	1.00	15.26	B
ATOM	2888	CA	GLU	B	6	18.295	14.932	-19.348	1.00	14.93	B
ATOM	2889	CB	GLU	B	6	19.563	14.057	-19.314	1.00	17.40	B
ATOM	2890	CG	GLU	B	6	19.320	12.568	-19.294	1.00	24.92	B
ATOM	2891	CD	GLU	B	6	20.397	11.849	-18.509	1.00	30.16	B
ATOM	2892	OE1	GLU	B	6	21.409	11.429	-19.117	1.00	31.47	B
ATOM	2893	OE2	GLU	B	6	20.235	11.721	-17.269	1.00	30.79	B
ATOM	2894	O	GLU	B	6	17.304	14.577	-18.204	1.00	14.96	B
ATOM	2895	O	GLU	B	6	17.478	14.983	-17.044	1.00	13.59	B
ATOM	2896	N	ARG	B	7	16.268	13.831	-18.547	1.00	13.17	B
ATOM	2897	CA	ARG	B	7	15.235	13.435	-17.595	1.00	13.08	B
ATOM	2898	CB	ARG	B	7	14.341	12.368	-18.216	1.00	12.64	B
ATOM	2899	CG	ARG	B	7	13.332	11.764	-17.240	1.00	11.85	B
ATOM	2900	CD	ARG	B	7	12.547	10.721	-17.988	1.00	14.66	B
ATOM	2901	NE	ARG	B	7	11.561	10.026	-17.142	1.00	13.57	B
ATOM	2902	CZ	ARG	B	7	11.809	8.942	-16.404	1.00	17.64	B
ATOM	2903	NH1	ARG	B	7	13.015	8.381	-16.365	1.00	17.50	B
ATOM	2904	NH2	ARG	B	7	10.839	8.391	-15.706	1.00	15.79	B
ATOM	2905	O	ARG	B	7	15.748	12.932	-16.243	1.00	14.94	B
ATOM	2906	O	ARG	B	7	15.326	13.421	-15.202	1.00	13.48	B
ATOM	2907	N	GLU	B	8	16.679	11.981	-16.256	1.00	15.15	B
ATOM	2908	CA	GLU	B	8	17.145	11.434	-14.973	1.00	18.15	B
ATOM	2909	CB	GLU	B	8	17.861	10.104	-15.238	1.00	18.04	B
ATOM	2910	CG	GLU	B	8	16.929	9.035	-15.849	1.00	19.35	B
ATOM	2911	CD	GLU	B	8	16.576	9.297	-17.297	1.00	17.91	B
ATOM	2912	OE1	GLU	B	8	17.433	9.801	-18.024	1.00	19.66	B
ATOM	2913	OE2	GLU	B	8	15.460	8.978	-17.745	1.00	18.19	B
ATOM	2914	O	GLU	B	8	17.988	12.368	-14.103	1.00	20.48	B
ATOM	2915	O	GLU	B	8	18.056	12.219	-12.878	1.00	19.63	B
ATOM	2916	N	HIS	B	9	18.613	13.364	-14.728	1.00	21.28	B
ATOM	2917	CA	HIS	B	9	19.426	14.333	-14.008	1.00	23.49	B
ATOM	2918	CB	HIS	B	9	20.297	15.041	-15.071	1.00	25.02	B
ATOM	2919	CG	HIS	B	9	21.522	15.711	-14.538	1.00	25.42	B
ATOM	2920	CD2	HIS	B	9	21.915	17.007	-14.589	1.00	28.09	B
ATOM	2921	ND1	HIS	B	9	22.466	15.056	-13.780	1.00	26.71	B
ATOM	2922	CE1	HIS	B	9	23.377	15.920	-13.367	1.00	27.14	B
ATOM	2923	NE2	HIS	B	9	23.064	17.114	-13.843	1.00	29.19	B
ATOM	2924	O	HIS	B	9	18.460	15.284	-13.250	1.00	22.99	B
ATOM	2925	O	HIS	B	9	18.789	15.913	-12.229	1.00	23.60	B
ATOM	2926	N	LEU	B	10	17.222	15.347	-13.737	1.00	21.72	B
ATOM	2927	CA	LEU	B	10	16.202	16.182	-13.157	1.00	21.01	B
ATOM	2928	CB	LEU	B	10	15.454	16.876	-14.310	1.00	21.10	B
ATOM	2929	CG	LEU	B	10	14.381	17.868	-13.903	1.00	19.07	B
ATOM	2930	CD1	LEU	B	10	15.051	19.052	-13.212	1.00	20.85	B
ATOM	2931	CD2	LEU	B	10	13.613	18.369	-15.152	1.00	18.56	B
ATOM	2932	O	LEU	B	10	15.181	15.513	-12.200	1.00	22.03	B
ATOM	2933	O	LEU	B	10	14.732	16.119	-11.216	1.00	23.32	B
ATOM	2934	N	LEU	B	11	14.860	14.247	-12.460	1.00	19.50	B
ATOM	2935	CA	LEU	B	11	13.848	13.520	-11.718	1.00	21.06	B
ATOM	2936	CB	LEU	B	11	13.667	12.159	-10.376	1.00	21.78	B
ATOM	2937	CG	LEU	B	11	12.270	11.573	-12.315	1.00	23.01	B
ATOM	2938	CD1	LEU	B	11	11.245	12.601	-12.812	1.00	26.14	B
ATOM	2939	CD2	LEU	B	11	12.219	10.366	-13.214	1.00	26.14	B
ATOM	2940	O	LEU	B	11	13.979	13.363	-10.192	1.00	21.79	B
ATOM	2941	O	LEU	B	11	13.053	13.717	-9.453	1.00	21.56	B
ATOM	2942	N	LYS	B	12	15.095	12.826	-9.717	1.00	23.82	B
ATOM	2943	CA	LYS	B	12	15.250	12.672	-8.267	1.00	24.71	B
ATOM	2944	CB	LYS	B	12	16.543	11.923	-7.915	1.00	28.61	B
ATOM	2945	CG	LYS	B	12	16.608	11.564	-6.431	1.00	31.97	B
ATOM	2946	CD	LYS	B	12	17.856	10.741	-6.085	1.00	36.79	B
ATOM	2947	CE	LYS	B	12	17.795	10.213	-4.650	1.00	37.65	B
ATOM	2948	NZ	LYS	B	12	17.449	11.262	-3.640	1.00	39.04	B
ATOM	2949	O	LYS	B	12	15.224	14.040	-7.576	1.00	22.39	B
ATOM	2950	O	LYS	B	12	14.586	14.193	-6.542	1.00	22.26	B
ATOM	2951	N	PRO	B	13	15.932	15.052	-8.123	1.00	20.35	B
ATOM	2952	CA	PRO	B	13	17.026	15.053	-9.103	1.00	19.55	B
ATOM	2953	CB	PRO	B	13	15.855	16.346	-7.434	1.00	19.49	B
ATOM	2954	CG	PRO	B	13	16.669	17.272	-8.333	1.00	19.36	B
ATOM	2955	CD	PRO	B	13	17.750	16.376	-8.827	1.00	19.86	B
ATOM	2956	O	PRO	B	13	14.420	16.838	-7.294	1.00	19.87	B
ATOM	2957	O	PRO	B	13	14.041	17.346	-6.250	1.00	17.95	B
ATOM	2958	N	LEU	B	14	13.620	16.710	-8.363	1.00	18.71	B
ATOM	2959	CA	LEU	B	14	12.231	17.130	-8.294	1.00	22.23	B
ATOM	2960	CB	LEU	B	14	11.532	16.907	-9.641	1.00	21.65	B
ATOM	2961	CG	LEU	B	14	11.656	17.995	-10.680	1.00	20.62	B
ATOM	2962	CD1	LEU	B	14	10.975	17.528	-11.993	1.00	18.11	B
ATOM	2963	CD2	LEU	B	14	11.024	19.287	-10.152	1.00	20.79	B
ATOM	2964	O	LEU	B	14	11.464	16.390	-7.215	1.00	22.60	B
ATOM	2965	O	LEU	B	14	10.644	16.963	-6.504	1.00	23.92	B

Figure 1 (continued 30)

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ATOM	2966	N	GLN	B	15	11.720	15.091	-7.121	1.00	24.48	B
ATOM	2967	CA	GLN	B	15	11.053	14.254	-6.149	1.00	25.57	B
ATOM	2968	CB	GLN	B	15	11.481	12.808	-6.340	1.00	28.51	B
ATOM	2969	CG	GLN	B	15	10.827	11.860	-5.383	1.00	32.34	B
ATOM	2970	CD	GLN	B	15	11.261	10.436	-5.657	1.00	35.26	B
ATOM	2971	OE1	GLN	B	15	11.086	9.924	-6.769	1.00	36.87	B
ATOM	2972	NE2	GLN	B	15	11.841	9.759	-4.651	1.00	27.81	B
ATOM	2973	C	GLN	B	15	11.402	14.692	-4.746	1.00	25.12	B
ATOM	2974	O	GLN	B	15	10.546	14.800	-3.872	1.00	24.87	B
ATOM	2975	N	GLN	B	16	12.685	14.941	-4.532	1.00	23.67	B
ATOM	2976	CA	GLN	B	16	13.133	15.374	-3.224	1.00	23.01	B
ATOM	2977	CB	GLN	B	16	14.649	15.351	-3.161	1.00	26.68	B
ATOM	2978	CG	GLN	B	16	15.220	13.938	-3.057	1.00	33.06	B
ATOM	2979	CD	GLN	B	16	15.149	13.363	-1.639	1.00	34.57	B
ATOM	2980	OE1	GLN	B	16	15.499	12.208	-1.417	1.00	37.92	B
ATOM	2981	NE2	GLN	B	16	14.709	14.170	-0.683	1.00	36.18	B
ATOM	2982	C	GLN	B	16	12.640	16.761	-2.798	1.00	22.25	B
ATOM	2983	O	GLN	B	16	12.218	16.966	-1.657	1.00	21.67	B
ATOM	2984	N	VAL	B	17	12.665	17.731	-3.697	1.00	19.74	B
ATOM	2985	CA	VAL	B	17	12.234	19.045	-3.234	1.00	21.71	B
ATOM	2986	CB	VAL	B	17	12.701	20.165	-4.175	1.00	21.43	B
ATOM	2987	CG1	VAL	B	17	14.229	20.161	-4.234	1.00	21.95	B
ATOM	2988	CG2	VAL	B	17	12.098	20.000	-5.563	1.00	17.76	B
ATOM	2989	C	VAL	B	17	10.738	19.160	-3.002	1.00	21.93	B
ATOM	2990	O	VAL	B	17	10.278	20.075	-2.330	1.00	23.73	B
ATOM	2991	N	SER	B	18	9.993	18.221	-3.545	1.00	23.91	B
ATOM	2992	CA	SER	B	18	8.548	18.205	-3.374	1.00	25.13	B
ATOM	2993	CB	SER	B	18	7.923	17.397	-4.502	1.00	25.03	B
ATOM	2994	CG	SER	B	18	8.075	18.078	-5.727	1.00	24.69	B
ATOM	2995	C	SER	B	18	8.092	17.636	-2.024	1.00	26.98	B
ATOM	2996	O	SER	B	18	6.926	17.771	-1.660	1.00	27.31	B
ATOM	2997	N	GLY	B	19	9.017	17.010	-1.300	1.00	26.53	B
ATOM	2998	CA	GLY	B	19	8.706	16.413	-0.012	1.00	27.63	B
ATOM	2999	CB	GLY	B	19	7.842	17.206	0.951	1.00	27.65	B
ATOM	3000	O	GLY	B	19	6.788	16.717	1.364	1.00	27.01	B
ATOM	3001	N	PRO	B	20	8.265	18.416	1.351	1.00	28.69	B
ATOM	3002	CA	PRO	B	20	9.611	18.974	1.119	1.00	30.14	B
ATOM	3003	CB	PRO	B	20	7.499	19.255	2.288	1.00	29.93	B
ATOM	3004	CG	PRO	B	20	8.462	20.415	2.594	1.00	30.20	B
ATOM	3005	C	PRO	B	20	9.415	20.424	1.436	1.00	30.31	B
ATOM	3006	O	PRO	B	20	6.111	19.744	1.848	1.00	31.66	B
ATOM	3007	N	PRO	B	20	5.360	20.297	2.650	1.00	32.04	B
ATOM	3008	CA	LEU	B	21	5.759	19.532	0.585	1.00	33.35	B
ATOM	3009	CB	LEU	B	21	4.456	19.982	0.089	1.00	34.98	B
ATOM	3010	CG	LEU	B	21	4.506	20.208	-1.429	1.00	33.56	B
ATOM	3011	CD	LEU	B	21	5.187	21.476	-1.954	1.00	33.69	B
ATOM	3012	OE1	LEU	B	21	6.657	21.499	-1.573	1.00	32.31	B
ATOM	3013	CD2	LEU	B	21	5.034	21.520	-3.473	1.00	33.19	B
ATOM	3014	C	LEU	B	21	3.331	19.003	0.412	1.00	36.25	B
ATOM	3015	O	LEU	B	21	3.543	17.799	0.452	1.00	37.14	B
ATOM	3016	N	GLY	B	22	2.132	19.540	0.636	1.00	38.77	B
ATOM	3017	CA	GLY	B	22	0.982	18.707	0.941	1.00	40.45	B
ATOM	3018	CB	GLY	B	22	0.122	18.423	-0.278	1.00	41.62	B
ATOM	3019	O	GLY	B	22	0.323	19.015	-1.348	1.00	42.14	B
ATOM	3020	N	GLY	B	23	-0.840	17.516	-0.117	1.00	42.36	B
ATOM	3021	CA	GLY	B	23	-1.731	17.170	-1.214	1.00	42.80	B
ATOM	3022	CB	GLY	B	23	-2.597	18.349	-1.621	1.00	42.52	B
ATOM	3023	O	GLY	B	23	-3.006	18.470	-2.776	1.00	42.78	B
ATOM	3024	N	ARG	B	24	-2.886	19.223	-0.664	1.00	42.28	B
ATOM	3025	CA	ARG	B	24	-3.691	20.400	-0.951	1.00	41.15	B
ATOM	3026	CB	ARG	B	24	-5.114	20.240	-0.419	1.00	44.69	B
ATOM	3027	CG	ARG	B	24	-6.032	21.311	-0.973	1.00	48.56	B
ATOM	3028	CD	ARG	B	24	-7.337	21.431	-0.212	1.00	52.31	B
ATOM	3029	NE	ARG	B	24	-8.207	22.431	-0.831	1.00	55.67	B
ATOM	3030	CZ	ARG	B	24	-7.851	23.690	-1.079	1.00	57.36	B
ATOM	3031	NH1	ARG	B	24	-6.634	24.122	-0.760	1.00	58.66	B
ATOM	3032	NH2	ARG	B	24	-8.711	24.521	-1.656	1.00	58.21	B
ATOM	3033	C	ARG	B	24	-3.067	21.645	-0.332	1.00	38.07	B
ATOM	3034	O	ARG	B	24	-3.273	21.934	0.845	1.00	38.01	B
ATOM	3035	N	PRO	B	25	-2.295	22.401	-1.124	1.00	35.11	B
ATOM	3036	CA	PRO	B	25	-2.021	22.244	-2.565	1.00	34.80	B
ATOM	3037	CB	PRO	B	25	-1.663	23.611	-0.601	1.00	32.06	B
ATOM	3038	CG	PRO	B	25	-0.820	24.099	-1.779	1.00	31.38	B
ATOM	3039	C	PRO	B	25	-1.619	23.646	-2.967	1.00	33.86	B
ATOM	3040	O	PRO	B	25	-2.692	24.634	-0.147	1.00	29.51	B
ATOM	3041	N	PRO	B	25	-3.711	24.864	-0.803	1.00	28.23	B
ATOM	3042	CA	THR	B	26	-2.412	25.236	0.996	1.00	28.41	B
ATOM	3043	CB	THR	B	26	-3.285	26.240	1.565	1.00	27.34	B
ATOM	3044	CG	THR	B	26	-2.673	26.752	2.861	1.00	28.45	B
ATOM	3045	CD	THR	B	26	-2.397	25.643	3.717	1.00	31.15	B
ATOM	3046	OE1	THR	B	26	-3.626	27.732	3.546	1.00	28.57	B
ATOM	3047	CD2	THR	B	26	-3.504	27.389	0.587	1.00	25.70	B
ATOM	3048	N	THR	B	26	-4.624	27.893	0.428	1.00	27.11	B
ATOM	3049	CA	LEU	B	27	-2.426	27.829	-0.044	1.00	23.09	B
ATOM	3050	CB	LEU	B	27	-2.507	28.881	-1.043	1.00	21.25	B
ATOM	3051	CG	LEU	B	27	-1.953	30.195	-0.531	1.00	21.63	B
ATOM	3052	C	LEU	B	27	-3.900	30.896	0.483	1.00	23.04	B
ATOM	3053	O	LEU	B	27	-2.264	32.203	0.895	1.00	24.85	B
ATOM	3054	N	LEU	B	27	-4.270	31.144	-0.160	1.00	24.74	B
ATOM	3055	CA	LEU	B	27	-1.718	28.392	-2.247	1.00	20.78	B
ATOM	3056	CB	LEU	B	27	-0.775	27.601	-2.105	1.00	17.68	B
ATOM	3057	CG	PRO	B	28	-2.084	28.863	-3.443	1.00	18.82	B
ATOM	3058	C	PRO	B	28	-3.104	29.903	-3.700	1.00	18.71	B
ATOM	3059	O	PRO	B	28	-1.413	28.443	-4.682	1.00	18.57	B
ATOM	3060	N	PRO	B	28	-1.917	29.446	-5.722	1.00	20.77	B
ATOM	3061	CA	PRO	B	28	-3.292	29.834	-5.195	1.00	20.10	B
ATOM	3062	CB	PRO	B	28	0.110	28.355	-4.684	1.00	18.35	B
ATOM	3063	O	PRO	B	28	0.666	27.322	-5.114	1.00	18.61	B
ATOM	3064	N	ILE	B	29	0.781	29.409	-4.230	1.00	16.22	B
ATOM	3065	CA	ILE	B	29	2.257	29.431	-4.241	1.00	17.45	B

Figure 1 (continued 31)

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ATOM	3066	CB	ILE	B	29	2.810	30.770	-3.637	1.00	19.27	B
ATOM	3067	CG2	ILE	B	29	2.555	30.812	-2.154	1.00	20.68	B
ATOM	3068	CG1	ILE	B	29	4.304	30.917	-3.901	1.00	23.27	B
ATOM	3069	CD1	ILE	B	29	4.653	31.204	-5.338	1.00	22.71	B
ATOM	3070	C	ILE	B	29	2.880	28.264	-3.502	1.00	15.97	B
ATOM	3071	O	ILE	B	29	3.957	27.778	-3.907	1.00	14.64	B
ATOM	3072	N	LEU	B	30	2.218	27.775	-2.452	1.00	16.95	B
ATOM	3073	CA	LEU	B	30	2.782	26.670	-1.664	1.00	16.78	B
ATOM	3074	CB	LEU	B	30	2.094	26.575	-0.300	1.00	18.79	B
ATOM	3075	CG	LEU	B	30	2.283	27.856	0.524	1.00	19.43	B
ATOM	3076	CD1	LEU	B	30	1.556	27.675	1.859	1.00	19.92	B
ATOM	3077	CD2	LEU	B	30	3.728	28.159	0.783	1.00	18.87	B
ATOM	3078	C	LEU	B	30	2.752	25.322	-2.374	1.00	17.78	B
ATOM	3079	O	LEU	B	30	3.343	24.340	-1.901	1.00	18.71	B
ATOM	3080	N	GLY	B	31	2.066	25.280	-3.505	1.00	14.09	B
ATOM	3081	CA	GLY	B	31	1.999	24.068	-4.318	1.00	15.57	B
ATOM	3082	C	GLY	B	31	2.992	24.160	-5.466	1.00	13.53	B
ATOM	3083	O	GLY	B	31	3.038	23.269	-6.317	1.00	15.55	B
ATOM	3084	N	ASN	B	32	3.796	25.200	-5.476	1.00	12.64	B
ATOM	3085	CA	ASN	B	32	4.767	25.400	-6.551	1.00	12.56	B
ATOM	3086	CB	ASN	B	32	4.690	26.838	-7.107	1.00	12.94	B
ATOM	3087	CG	ASN	B	32	3.502	27.045	-8.024	1.00	10.96	B
ATOM	3088	OD1	ASN	B	32	2.599	26.224	-8.085	1.00	12.20	B
ATOM	3089	ND2	ASN	B	32	3.523	28.158	-8.771	1.00	13.16	B
ATOM	3090	C	ASN	B	32	6.178	25.176	-6.075	1.00	14.19	B
ATOM	3091	O	ASN	B	32	6.481	25.195	-4.868	1.00	14.24	B
ATOM	3092	N	LEU	B	33	7.050	24.957	-7.052	1.00	13.85	B
ATOM	3093	CA	LEU	B	33	8.459	24.861	-6.774	1.00	13.97	B
ATOM	3094	CB	LEU	B	33	9.097	23.641	-7.433	1.00	15.40	B
ATOM	3095	CG	LEU	B	33	8.586	22.254	-7.072	1.00	17.90	B
ATOM	3096	CD1	LEU	B	33	9.410	21.226	-7.867	1.00	18.49	B
ATOM	3097	CD2	LEU	B	33	8.782	22.024	-5.568	1.00	19.70	B
ATOM	3098	C	LEU	B	33	9.115	26.086	-7.395	1.00	13.05	B
ATOM	3099	O	LEU	B	33	8.725	26.540	-8.465	1.00	13.07	B
ATOM	3100	N	LEU	B	34	10.126	26.610	-6.722	1.00	12.75	B
ATOM	3101	CA	LEU	B	34	10.895	27.732	-7.225	1.00	12.14	B
ATOM	3102	CB	LEU	B	34	11.510	28.520	-6.056	1.00	13.47	B
ATOM	3103	CG	LEU	B	34	12.562	29.560	-6.427	1.00	12.92	B
ATOM	3104	CD1	LEU	B	34	11.973	30.697	-7.293	1.00	14.04	B
ATOM	3105	CD2	LEU	B	34	13.130	30.156	-5.123	1.00	14.82	B
ATOM	3106	C	LEU	B	34	12.029	27.176	-8.099	1.00	13.14	B
ATOM	3107	O	LEU	B	34	12.760	26.275	-7.652	1.00	12.90	B
ATOM	3108	N	LEU	B	35	12.125	27.651	-9.351	1.00	11.64	B
ATOM	3109	CA	LEU	B	35	13.187	27.245	-10.291	1.00	11.91	B
ATOM	3110	CB	LEU	B	35	12.615	26.811	-11.669	1.00	11.42	B
ATOM	3111	CG	LEU	B	35	12.046	25.413	-11.738	1.00	14.74	B
ATOM	3112	CD1	LEU	B	35	11.127	25.120	-10.596	1.00	18.38	B
ATOM	3113	CD2	LEU	B	35	11.288	25.299	-13.074	1.00	15.91	B
ATOM	3114	C	LEU	B	35	14.071	28.445	-10.542	1.00	13.47	B
ATOM	3115	O	LEU	B	35	13.573	29.535	-10.900	1.00	14.51	B
ATOM	3116	N	GLN	B	36	15.376	28.285	-10.350	1.00	13.11	B
ATOM	3117	CA	GLN	B	36	16.300	29.400	-10.578	1.00	13.83	B
ATOM	3118	CB	GLN	B	36	16.806	29.935	-9.223	1.00	16.13	B
ATOM	3119	CG	GLN	B	36	15.726	30.383	-8.281	1.00	16.86	B
ATOM	3120	CD	GLN	B	36	16.264	30.626	-6.866	1.00	21.26	B
ATOM	3121	OE1	GLN	B	36	16.232	31.760	-6.363	1.00	25.16	B
ATOM	3122	NE2	GLN	B	36	16.770	29.570	-6.229	1.00	16.45	B
ATOM	3123	C	GLN	B	36	17.495	28.935	-11.376	1.00	13.60	B
ATOM	3124	O	GLN	B	36	18.135	27.952	-10.997	1.00	14.49	B
ATOM	3125	N	VAL	B	37	17.810	29.640	-12.474	1.00	11.56	B
ATOM	3126	CA	VAL	B	37	18.997	29.285	-13.248	1.00	13.61	B
ATOM	3127	CB	VAL	B	37	18.731	29.191	-14.777	1.00	12.84	B
ATOM	3128	CG1	VAL	B	37	20.074	29.020	-15.553	1.00	14.43	B
ATOM	3129	CG2	VAL	B	37	17.804	27.985	-15.051	1.00	14.23	B
ATOM	3130	C	VAL	B	37	19.265	30.435	-13.005	1.00	15.18	B
ATOM	3131	O	VAL	B	37	19.611	31.603	-13.228	1.00	15.34	B
ATOM	3132	N	ALA	B	38	21.139	30.117	-12.472	1.00	15.02	B
ATOM	3133	CA	ALA	B	38	22.161	31.146	-12.227	1.00	15.51	B
ATOM	3134	CB	ALA	B	38	21.954	31.783	-10.878	1.00	15.09	B
ATOM	3135	C	ALA	B	38	23.493	30.446	-12.291	1.00	19.33	B
ATOM	3136	O	ALA	B	38	23.644	29.366	-11.747	1.00	18.26	B
ATOM	3137	N	ASP	B	39	24.473	31.060	-12.953	1.00	22.66	B
ATOM	3138	CA	ASP	B	39	25.765	30.393	-13.153	1.00	26.58	B
ATOM	3139	CB	ASP	B	39	26.389	29.982	-11.829	1.00	32.37	B
ATOM	3140	CG	ASP	B	39	27.184	31.097	-11.201	1.00	36.57	B
ATOM	3141	OD1	ASP	B	39	28.336	31.328	-11.655	1.00	39.34	B
ATOM	3142	OD2	ASP	B	39	26.658	31.756	-10.270	1.00	38.78	B
ATOM	3143	C	ASP	B	39	25.429	29.150	-13.986	1.00	26.82	B
ATOM	3144	O	ASP	B	39	24.550	29.189	-14.844	1.00	29.26	B
ATOM	3145	N	GLY	B	40	26.080	28.031	-13.733	1.00	26.59	B
ATOM	3146	CA	GLY	B	40	25.759	26.871	-14.539	1.00	23.64	B
ATOM	3147	C	GLY	B	40	24.910	25.927	-13.730	1.00	19.76	B
ATOM	3148	O	GLY	B	40	25.044	24.723	-13.871	1.00	20.20	B
ATOM	3149	N	THR	B	41	24.046	26.498	-12.883	1.00	18.09	B
ATOM	3150	CA	THR	B	41	23.215	25.701	-11.983	1.00	15.70	B
ATOM	3151	CB	THR	B	41	23.684	25.916	-10.551	1.00	16.47	B
ATOM	3152	OG1	THR	B	41	25.090	25.633	-10.486	1.00	19.61	B
ATOM	3153	CG2	THR	B	41	22.918	25.016	-9.549	1.00	17.43	B
ATOM	3154	C	THR	B	41	21.721	25.988	-11.974	1.00	13.03	B
ATOM	3155	O	THR	B	41	21.308	27.129	-11.944	1.00	14.12	B
ATOM	3156	N	LEU	B	42	20.924	24.933	-12.005	1.00	13.26	B
ATOM	3157	CA	LEU	B	42	19.483	25.093	-11.850	1.00	11.94	B
ATOM	3158	CB	LEU	B	42	18.743	24.061	-12.723	1.00	11.39	B
ATOM	3159	CG	LEU	B	42	17.292	23.803	-12.339	1.00	10.89	B
ATOM	3160	CD1	LEU	B	42	16.422	25.083	-12.504	1.00	13.06	B
ATOM	3161	CD2	LEU	B	42	16.760	22.694	-13.241	1.00	12.39	B
ATOM	3162	C	LEU	B	42	19.222	24.731	-10.385	1.00	12.70	B
ATOM	3163	O	LEU	B	42	19.633	23.642	-9.935	1.00	13.40	B
ATOM	3164	N	SER	B	43	18.551	25.613	-9.641	1.00	10.83	B
ATOM	3165	CA	SER	B	43	18.212	25.317	-8.240	1.00	13.03	B

Figure 1 (continued 32)

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ATOM	3166	CB	SER	B	43	18.605	26.457	-7.298	1.00	15.48	B
ATOM	3167	O	SER	B	43	20.017	26.635	-7.258	1.00	16.36	B
ATOM	3168	O	SER	B	43	16.699	25.141	-8.194	1.00	12.37	B
ATOM	3169	O	SER	B	43	15.953	25.873	-8.875	1.00	13.81	B
ATOM	3170	N	LEU	B	44	16.259	24.133	-7.427	1.00	12.48	B
ATOM	3171	CA	LEU	B	44	14.832	23.840	-7.249	1.00	11.34	B
ATOM	3172	CB	LEU	B	44	14.504	22.413	-7.724	1.00	12.56	B
ATOM	3173	CG	LEU	B	44	14.993	22.028	-9.122	1.00	14.70	B
ATOM	3174	CD1	LEU	B	44	14.964	20.500	-9.306	1.00	18.40	B
ATOM	3175	CD2	LEU	B	44	14.105	22.717	-10.133	1.00	19.25	B
ATOM	3176	C	LEU	B	44	14.581	23.918	-5.746	1.00	13.84	B
ATOM	3177	O	LEU	B	44	15.344	23.356	-4.936	1.00	12.96	B
ATOM	3178	N	THR	B	45	13.499	24.583	-5.359	1.00	11.87	B
ATOM	3179	CA	THR	B	45	13.179	24.726	-3.928	1.00	13.31	B
ATOM	3180	CB	THR	B	45	13.481	26.166	-3.421	1.00	13.75	B
ATOM	3181	OG1	THR	B	45	14.869	26.488	-1.627	1.00	15.13	B
ATOM	3182	CG2	THR	B	45	13.157	26.269	-1.322	1.00	14.06	B
ATOM	3183	C	THR	B	45	11.698	24.477	-3.666	1.00	14.00	B
ATOM	3184	O	THR	B	45	10.867	24.948	-4.423	1.00	13.55	B
ATOM	3185	N	GLY	B	46	11.396	23.696	-2.631	1.00	13.22	B
ATOM	3186	CA	GLY	B	46	10.029	23.408	-2.203	1.00	14.39	B
ATOM	3187	C	GLY	B	46	9.898	23.843	-0.738	1.00	15.56	B
ATOM	3188	O	GLY	B	46	10.856	23.711	0.017	1.00	14.57	B
ATOM	3189	N	THR	B	47	8.736	24.387	-0.333	1.00	15.34	B
ATOM	3190	CA	THR	B	47	8.592	24.822	1.061	1.00	16.19	B
ATOM	3191	CB	THR	B	47	8.985	26.317	1.236	1.00	15.79	B
ATOM	3192	OG1	THR	B	47	9.049	26.655	2.632	1.00	17.31	B
ATOM	3193	CG2	THR	B	47	7.967	27.253	0.564	1.00	16.59	B
ATOM	3194	C	THR	B	47	7.162	24.668	1.564	1.00	16.42	B
ATOM	3195	O	THR	B	47	6.226	24.562	0.768	1.00	17.13	B
ATOM	3196	N	ASP	B	48	7.009	24.615	2.887	1.00	16.11	B
ATOM	3197	CA	ASP	B	48	5.658	24.598	3.487	1.00	15.80	B
ATOM	3198	CB	ASP	B	48	5.344	23.244	4.132	1.00	16.28	B
ATOM	3199	CG	ASP	B	48	6.136	22.986	5.398	1.00	16.79	B
ATOM	3200	OD1	ASP	B	48	7.041	23.773	5.722	1.00	20.58	B
ATOM	3201	OD2	ASP	B	48	5.825	21.976	6.074	1.00	18.07	B
ATOM	3202	C	ASP	B	48	5.559	25.736	4.521	1.00	18.39	B
ATOM	3203	O	ASP	B	48	4.612	25.768	5.321	1.00	15.86	B
ATOM	3204	N	LEU	B	49	6.545	26.641	4.479	1.00	17.77	B
ATOM	3205	CA	LEU	B	49	6.712	27.827	5.343	1.00	17.51	B
ATOM	3206	CB	LEU	B	49	5.383	28.520	5.666	1.00	17.64	B
ATOM	3207	CG	LEU	B	49	4.676	29.110	4.453	1.00	21.50	B
ATOM	3208	CD1	LEU	B	49	3.373	29.816	4.956	1.00	19.20	B
ATOM	3209	CD2	LEU	B	49	5.594	30.102	3.756	1.00	16.84	B
ATOM	3210	C	LEU	B	49	7.406	27.475	6.656	1.00	20.06	B
ATOM	3211	O	LEU	B	49	7.860	28.372	7.370	1.00	17.57	B
ATOM	3212	N	GLU	B	50	7.467	26.189	6.991	1.00	16.55	B
ATOM	3213	CA	GLU	B	50	8.164	25.802	8.228	1.00	20.80	B
ATOM	3214	CB	GLU	B	50	7.359	24.747	9.000	1.00	25.34	B
ATOM	3215	CG	GLU	B	50	7.969	24.377	10.373	1.00	29.02	B
ATOM	3216	CD	GLU	B	50	7.109	23.396	11.186	1.00	30.09	B
ATOM	3217	OE1	GLU	B	50	7.079	23.504	12.435	1.00	31.29	B
ATOM	3218	OE2	GLU	B	50	6.487	22.496	10.592	1.00	16.32	B
ATOM	3219	O	GLU	B	50	9.540	25.238	7.842	1.00	16.99	B
ATOM	3220	C	GLU	B	50	10.511	25.373	8.580	1.00	15.47	B
ATOM	3221	N	MET	B	51	9.611	24.630	6.672	1.00	14.90	B
ATOM	3222	CA	MET	B	51	10.882	24.074	6.215	1.00	15.67	B
ATOM	3223	CB	MET	B	51	10.987	22.609	6.653	1.00	17.25	B
ATOM	3224	CG	MET	B	51	9.910	21.720	6.114	1.00	21.05	B
ATOM	3225	CD	MET	B	51	9.719	20.228	7.113	1.00	23.10	B
ATOM	3226	OE1	MET	B	51	8.965	20.945	8.604	1.00	14.86	B
ATOM	3227	OE2	MET	B	51	10.988	24.187	4.721	1.00	15.26	B
ATOM	3228	C	MET	B	51	9.978	24.437	4.029	1.00	14.83	B
ATOM	3229	O	GLU	B	52	12.210	24.027	4.202	1.00	13.34	B
ATOM	3230	N	GLU	B	52	12.367	24.087	2.755	1.00	18.93	B
ATOM	3231	CA	GLU	B	52	12.761	25.477	2.295	1.00	25.39	B
ATOM	3232	CB	GLU	B	52	13.998	26.005	2.925	1.00	31.84	B
ATOM	3233	CG	GLU	B	52	14.361	27.374	2.411	1.00	32.96	B
ATOM	3234	CD	GLU	B	52	13.504	28.295	2.473	1.00	35.26	B
ATOM	3235	OE1	GLU	B	52	15.520	27.508	1.960	1.00	14.63	B
ATOM	3236	OE2	GLU	B	52	13.420	23.100	2.339	1.00	14.47	B
ATOM	3237	C	GLU	B	52	14.317	22.798	3.108	1.00	13.33	B
ATOM	3238	N	MET	B	53	13.314	22.604	1.117	1.00	14.02	B
ATOM	3239	CA	MET	B	53	14.280	21.636	0.610	1.00	16.35	B
ATOM	3240	CB	MET	B	53	13.575	20.289	0.379	1.00	19.16	B
ATOM	3241	CG	MET	B	53	14.496	19.209	-0.220	1.00	23.65	B
ATOM	3242	CD	MET	B	53	15.833	18.696	0.914	1.00	20.87	B
ATOM	3243	OE1	MET	B	53	14.878	17.649	1.951	1.00	14.06	B
ATOM	3244	OE2	MET	B	53	14.777	22.225	-0.701	1.00	13.90	B
ATOM	3245	C	MET	B	53	13.977	22.607	-1.546	1.00	13.10	B
ATOM	3246	N	VAL	B	54	16.091	22.294	-0.872	1.00	13.22	B
ATOM	3247	CA	VAL	B	54	16.687	22.882	-2.089	1.00	14.45	B
ATOM	3248	CB	VAL	B	54	17.539	24.079	-1.725	1.00	14.52	B
ATOM	3249	CG1	VAL	B	54	18.117	24.704	-2.984	1.00	13.15	B
ATOM	3250	CG2	VAL	B	54	16.699	25.088	-0.938	1.00	13.82	B
ATOM	3251	C	VAL	B	54	17.590	21.867	-2.768	1.00	16.01	B
ATOM	3252	O	VAL	B	54	18.330	21.169	-2.093	1.00	11.25	B
ATOM	3253	N	ALA	B	55	17.513	21.765	-4.096	1.00	13.21	B
ATOM	3254	CA	ALA	B	55	18.380	20.865	-4.850	1.00	12.81	B
ATOM	3255	CB	ALA	B	55	17.548	19.820	-5.605	1.00	15.53	B
ATOM	3256	C	ALA	B	55	19.144	21.706	-5.863	1.00	15.73	B
ATOM	3257	O	ALA	B	55	18.564	22.606	-6.461	1.00	14.23	B
ATOM	3258	N	ARG	B	56	20.433	21.410	-6.059	1.00	15.31	B
ATOM	3259	CA	ARG	B	56	21.258	22.119	-7.044	1.00	16.38	B
ATOM	3260	CB	ARG	B	56	22.601	22.523	-6.432	1.00	22.20	B
ATOM	3261	CG	ARG	B	56	22.482	23.229	-5.112	1.00	24.40	B
ATOM	3262	CD	ARG	B	56	22.101	24.643	-5.283	1.00	26.52	B
ATOM	3263	NE	ARG	B	56	22.131	25.327	-3.990	1.00	27.62	B
ATOM	3264	CZ	ARG	B	56	21.494	26.463	-3.729	1.00	23.46	B
ATOM	3265	NH1	ARG	B	56	20.779	27.069	-4.676	1.00		B

Figure 1 (continued 33)

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ATOM	3266	NH2	ARG	B	56	21.523	26.966	-2.496	1.00	28.24	B
ATOM	3267	C	ARG	B	56	21.525	21.120	-8.158	1.00	14.84	B
ATOM	3268	O	ARG	B	56	21.995	19.996	-7.905	1.00	16.83	B
ATOM	3269	N	VAL	B	57	21.203	21.504	-9.387	1.00	13.57	B
ATOM	3270	CA	VAL	B	57	21.402	20.616	-10.511	1.00	15.14	B
ATOM	3271	CB	VAL	B	57	20.049	20.326	-11.197	1.00	17.22	B
ATOM	3272	CG1	VAL	B	57	20.238	19.426	-12.403	1.00	17.28	B
ATOM	3273	CG2	VAL	B	57	19.076	19.642	-10.185	1.00	16.94	B
ATOM	3274	C	VAL	B	57	22.378	21.261	-11.510	1.00	14.02	B
ATOM	3275	O	VAL	B	57	22.090	22.326	-12.063	1.00	15.02	B
ATOM	3276	N	ALA	B	58	23.495	20.589	-11.786	1.00	15.91	B
ATOM	3277	CA	ALA	B	58	24.457	21.141	-12.749	1.00	15.97	B
ATOM	3278	CB	ALA	B	58	25.763	20.328	-12.705	1.00	16.60	B
ATOM	3279	C	ALA	B	58	23.883	21.096	-14.178	1.00	15.88	B
ATOM	3280	O	ALA	B	58	23.266	20.118	-14.569	1.00	16.91	B
ATOM	3281	N	LEU	B	59	24.106	22.157	-14.947	1.00	13.80	B
ATOM	3282	CA	LEU	B	59	23.618	22.249	-16.321	1.00	13.84	B
ATOM	3283	CB	LEU	B	59	22.888	23.587	-16.527	1.00	14.79	B
ATOM	3284	CG	LEU	B	59	21.708	23.860	-15.578	1.00	13.18	B
ATOM	3285	CD1	LEU	B	59	21.112	25.257	-15.826	1.00	16.02	B
ATOM	3286	CD2	LEU	B	59	20.641	22.815	-15.803	1.00	13.77	B
ATOM	3287	C	LEU	B	59	24.820	22.178	-17.264	1.00	16.59	B
ATOM	3288	O	LEU	B	59	25.670	23.089	-17.254	1.00	18.41	B
ATOM	3289	N	VAL	B	60	24.906	21.089	-18.037	1.00	16.00	B
ATOM	3290	CA	VAL	B	60	25.987	20.866	-19.030	1.00	16.12	B
ATOM	3291	CB	VAL	B	60	26.497	19.402	-19.011	1.00	17.87	B
ATOM	3292	CG1	VAL	B	60	27.080	19.074	-17.627	1.00	17.15	B
ATOM	3293	CG2	VAL	B	60	25.361	18.434	-19.397	1.00	15.97	B
ATOM	3294	C	VAL	B	60	25.541	21.219	-20.443	1.00	18.35	B
ATOM	3295	O	VAL	B	60	26.366	21.214	-21.382	1.00	18.50	B
ATOM	3296	N	GLN	B	61	24.259	21.561	-20.617	1.00	17.91	B
ATOM	3297	CA	GLN	B	61	23.731	21.970	-21.926	1.00	18.15	B
ATOM	3298	CB	GLN	B	61	22.400	21.256	-22.242	1.00	17.50	B
ATOM	3299	CG	GLN	B	61	22.541	19.751	-22.248	1.00	17.69	B
ATOM	3300	CD	GLN	B	61	21.298	19.043	-22.798	1.00	14.84	B
ATOM	3301	OE1	GLN	B	61	20.828	19.336	-23.922	1.00	16.87	B
ATOM	3302	NE2	GLN	B	61	20.776	18.097	-22.026	1.00	16.99	B
ATOM	3303	C	GLN	B	61	23.478	23.468	-21.873	1.00	19.28	B
ATOM	3304	O	GLN	B	61	23.366	24.036	-20.778	1.00	17.31	B
ATOM	3305	N	PRO	B	62	23.351	24.125	-23.046	1.00	18.68	B
ATOM	3306	CD	PRO	B	62	23.472	23.548	-24.401	1.00	20.65	B
ATOM	3307	CA	PRO	B	62	23.098	25.577	-23.114	1.00	19.82	B
ATOM	3308	CB	PRO	B	62	22.828	25.809	-24.591	1.00	22.37	B
ATOM	3309	CG	PRO	B	62	23.740	24.781	-25.242	1.00	21.05	B
ATOM	3310	C	PRO	B	62	21.934	26.045	-22.220	1.00	19.61	B
ATOM	3311	O	PRO	B	62	20.901	25.388	-22.159	1.00	19.83	B
ATOM	3312	N	HIS	B	63	22.121	27.174	-21.533	1.00	16.71	B
ATOM	3313	CA	HIS	B	63	21.102	27.720	-20.624	1.00	15.04	B
ATOM	3314	CB	HIS	B	63	21.307	27.117	-19.223	1.00	16.87	B
ATOM	3315	CG	HIS	B	63	22.718	27.225	-18.743	1.00	16.35	B
ATOM	3316	CD2	HIS	B	63	23.352	28.194	-18.045	1.00	19.97	B
ATOM	3317	ND1	HIS	B	63	23.674	26.284	-19.052	1.00	19.14	B
ATOM	3318	CE1	HIS	B	63	24.844	26.671	-18.566	1.00	18.64	B
ATOM	3319	NE2	HIS	B	63	24.676	27.828	-17.954	1.00	21.06	B
ATOM	3320	C	HIS	B	63	21.120	29.242	-20.524	1.00	16.64	B
ATOM	3321	O	HIS	B	63	22.102	29.903	-20.917	1.00	18.95	B
ATOM	3322	N	GLU	B	64	20.043	29.811	-19.988	1.00	14.93	B
ATOM	3323	CA	GLU	B	64	19.904	31.269	-19.792	1.00	16.90	B
ATOM	3324	CB	GLU	B	64	18.948	31.878	-20.827	1.00	20.34	B
ATOM	3325	CG	GLU	B	64	19.523	31.891	-22.209	1.00	23.46	B
ATOM	3326	CD	GLU	B	64	18.491	32.235	-23.268	1.00	28.27	B
ATOM	3327	OE1	GLU	B	64	17.465	32.858	-22.936	1.00	28.18	B
ATOM	3328	OE2	GLU	B	64	18.725	31.878	-24.441	1.00	30.88	B
ATOM	3329	C	GLU	B	64	19.369	31.526	-18.386	1.00	16.81	B
ATOM	3330	O	GLU	B	64	18.451	30.834	-17.941	1.00	16.15	B
ATOM	3331	N	PRO	B	65	19.945	32.500	-17.653	1.00	15.86	B
ATOM	3332	CD	PRO	B	65	21.078	33.356	-18.046	1.00	17.72	B
ATOM	3333	CA	PRO	B	65	19.502	32.808	-16.292	1.00	15.04	B
ATOM	3334	CB	PRO	B	65	20.587	33.780	-15.774	1.00	17.31	B
ATOM	3335	CG	PRO	B	65	21.018	34.457	-16.991	1.00	18.09	B
ATOM	3336	C	PRO	B	65	18.088	33.355	-16.113	1.00	15.66	B
ATOM	3337	O	PRO	B	65	17.508	33.964	-17.024	1.00	16.81	B
ATOM	3338	N	GLY	B	66	17.530	33.112	-14.930	1.00	14.69	B
ATOM	3339	CA	GLY	B	66	16.200	33.578	-14.601	1.00	14.85	B
ATOM	3340	C	GLY	B	66	15.477	32.710	-13.600	1.00	15.33	B
ATOM	3341	O	GLY	B	66	16.001	31.653	-13.195	1.00	14.73	B
ATOM	3342	N	ALA	B	67	14.286	33.140	-13.187	1.00	13.47	B
ATOM	3343	CA	ALA	B	67	13.542	32.384	-12.182	1.00	14.65	B
ATOM	3344	CB	ALA	B	67	13.917	32.882	-10.767	1.00	14.42	B
ATOM	3345	C	ALA	B	67	12.054	32.455	-12.334	1.00	14.70	B
ATOM	3346	O	ALA	B	67	11.505	33.439	-12.854	1.00	15.40	B
ATOM	3347	N	THR	B	68	11.386	31.417	-11.857	1.00	13.62	B
ATOM	3348	CA	THR	B	68	9.929	31.390	-11.878	1.00	13.91	B
ATOM	3349	CB	THR	B	68	9.391	31.110	-13.317	1.00	14.48	B
ATOM	3350	OG1	THR	B	68	7.963	31.295	-13.339	1.00	15.83	B
ATOM	3351	CG2	THR	B	68	9.694	29.668	-13.731	1.00	16.00	B
ATOM	3352	C	THR	B	68	9.472	30.302	-10.924	1.00	14.71	B
ATOM	3353	O	THR	B	68	10.311	29.641	-10.323	1.00	15.32	B
ATOM	3354	N	THR	B	69	8.167	30.162	-10.724	1.00	13.55	B
ATOM	3355	CA	THR	B	69	7.636	29.056	-9.894	1.00	12.29	B
ATOM	3356	CB	THR	B	69	7.048	29.522	-8.520	1.00	14.79	B
ATOM	3357	OG1	THR	B	69	5.754	30.105	-8.695	1.00	15.03	B
ATOM	3358	CG2	THR	B	69	7.983	30.537	-7.876	1.00	14.41	B
ATOM	3359	C	THR	B	69	6.555	28.385	-10.714	1.00	14.44	B
ATOM	3360	O	THR	B	69	5.847	29.055	-11.465	1.00	14.38	B
ATOM	3361	N	VAL	B	70	6.458	27.063	-10.629	1.00	13.03	B
ATOM	3362	CA	VAL	B	70	5.464	26.297	-11.370	1.00	12.62	B
ATOM	3363	CB	VAL	B	70	6.044	25.655	-12.631	1.00	14.60	B
ATOM	3364	CG1	VAL	B	70	6.340	26.733	-13.667	1.00	17.68	B
ATOM	3365	CG2	VAL	B	70	7.284	24.840	-12.267	1.00	16.64	B

Figure 1 (continued 34)

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ATOM	3366	C	VAL	B	70	4.913	25.183	-10.490	1.00	12.72	B
ATOM	3367	O	VAL	B	70	5.550	24.803	-9.489	1.00	12.07	B
ATOM	3368	N	PRO	B	71	3.734	24.651	-10.825	1.00	12.89	B
ATOM	3369	CD	PRO	B	71	2.872	25.050	-11.964	1.00	14.31	B
ATOM	3370	CA	PRO	B	71	3.129	23.572	-10.016	1.00	12.87	B
ATOM	3371	CB	PRO	B	71	1.845	23.239	-10.756	1.00	14.80	B
ATOM	3372	CG	PRO	B	71	1.522	24.614	-11.481	1.00	19.52	B
ATOM	3373	C	PRO	B	71	4.044	22.363	-9.848	1.00	12.82	B
ATOM	3374	O	PRO	B	71	4.480	21.743	-10.813	1.00	13.40	B
ATOM	3375	N	ALA	B	72	4.340	22.035	-8.599	1.00	11.96	B
ATOM	3376	CA	ALA	B	72	5.293	20.944	-8.344	1.00	11.56	B
ATOM	3377	CB	ALA	B	72	5.611	20.907	-6.847	1.00	12.77	B
ATOM	3378	C	ALA	B	72	4.857	19.587	-8.805	1.00	13.14	B
ATOM	3379	O	ALA	B	72	5.618	18.899	-9.515	1.00	11.71	B
ATOM	3380	N	ARG	B	73	3.654	19.178	-8.426	1.00	12.89	B
ATOM	3381	CA	ARG	B	73	3.155	17.856	-8.777	1.00	15.37	B
ATOM	3382	CB	ARG	B	73	1.769	17.634	-8.137	1.00	19.29	B
ATOM	3383	CG	ARG	B	73	1.189	16.241	-8.362	1.00	28.52	B
ATOM	3384	CD	ARG	B	73	2.091	15.198	-7.713	1.00	33.56	B
ATOM	3385	NE	ARG	B	73	1.915	13.882	-8.310	1.00	39.25	B
ATOM	3386	CZ	ARG	B	73	2.786	12.882	-8.182	1.00	39.95	B
ATOM	3387	NH1	ARG	B	73	3.894	13.052	-7.476	1.00	40.90	B
ATOM	3388	NH2	ARG	B	73	2.549	11.711	-8.772	1.00	41.65	B
ATOM	3389	C	ARG	B	73	3.074	17.695	-10.292	1.00	12.85	B
ATOM	3390	O	ARG	B	73	3.480	16.668	-10.851	1.00	12.28	B
ATOM	3391	N	LYS	B	74	2.530	18.708	-10.956	1.00	12.56	B
ATOM	3392	CA	LYS	B	74	2.387	18.655	-12.419	1.00	12.58	B
ATOM	3393	CB	LYS	B	74	1.647	19.886	-12.933	1.00	11.93	B
ATOM	3394	CG	LYS	B	74	0.149	19.815	-12.596	1.00	13.85	B
ATOM	3395	CD	LYS	B	74	-0.493	21.183	-12.811	1.00	15.33	B
ATOM	3396	CE	LYS	B	74	-1.982	21.112	-12.597	1.00	16.90	B
ATOM	3397	CZ	LYS	B	74	-2.482	22.535	-12.538	1.00	17.31	B
ATOM	3398	C	LYS	B	74	3.729	18.561	-13.101	1.00	11.10	B
ATOM	3399	O	LYS	B	74	3.882	17.738	-14.009	1.00	11.83	B
ATOM	3400	N	PHE	B	75	4.697	19.379	-12.673	1.00	11.16	B
ATOM	3401	CA	PHE	B	75	6.015	19.357	-13.326	1.00	8.77	B
ATOM	3402	CB	PHE	B	75	6.951	20.553	-12.366	1.00	9.59	B
ATOM	3403	CG	PHE	B	75	8.199	20.686	-13.568	1.00	11.61	B
ATOM	3404	CD1	PHE	B	75	8.300	20.587	-14.956	1.00	12.29	B
ATOM	3405	CD2	PHE	B	75	9.320	20.975	-12.835	1.00	12.93	B
ATOM	3406	CE1	PHE	B	75	9.567	20.783	-15.596	1.00	14.18	B
ATOM	3407	CE2	PHE	B	75	10.561	21.172	-13.448	1.00	16.28	B
ATOM	3408	CZ	PHE	B	75	10.677	21.069	-14.836	1.00	13.85	B
ATOM	3409	C	PHE	B	75	6.699	18.029	-13.066	1.00	10.84	B
ATOM	3410	O	PHE	B	75	7.225	17.420	-14.009	1.00	9.16	B
ATOM	3411	N	PHE	B	76	6.663	17.552	-11.819	1.00	10.39	B
ATOM	3412	CA	PHE	B	76	7.252	16.230	-11.555	1.00	11.16	B
ATOM	3413	CB	PHE	B	76	7.138	15.862	-10.092	1.00	12.22	B
ATOM	3414	CG	PHE	B	76	7.546	14.459	-9.823	1.00	14.40	B
ATOM	3415	CD1	PHE	B	76	8.888	14.117	-9.730	1.00	16.66	B
ATOM	3416	CD2	PHE	B	76	6.583	13.475	-9.667	1.00	16.99	B
ATOM	3417	CE1	PHE	B	76	9.252	12.795	-9.461	1.00	17.02	B
ATOM	3418	CE2	PHE	B	76	6.946	12.143	-9.407	1.00	17.99	B
ATOM	3419	CZ	PHE	B	76	8.275	11.821	-9.302	1.00	18.48	B
ATOM	3420	C	PHE	B	76	6.579	15.133	-12.373	1.00	12.82	B
ATOM	3421	O	PHE	B	76	7.255	14.307	-12.999	1.00	10.50	B
ATOM	3422	N	ASP	B	77	5.247	15.103	-12.399	1.00	10.55	B
ATOM	3423	CA	ASP	B	77	4.563	14.074	-13.173	1.00	9.78	B
ATOM	3424	CB	ASP	B	77	3.053	14.178	-12.970	1.00	11.78	B
ATOM	3425	CG	ASP	B	77	2.626	13.732	-11.596	1.00	17.39	B
ATOM	3426	OD1	ASP	B	77	3.429	13.121	-10.843	1.00	17.35	B
ATOM	3427	OD2	ASP	B	77	1.441	13.973	-11.260	1.00	18.13	B
ATOM	3428	C	ASP	B	77	4.893	14.113	-14.663	1.00	8.50	B
ATOM	3429	O	ASP	B	77	5.004	13.055	-15.288	1.00	10.06	B
ATOM	3430	N	ILE	B	78	5.065	15.316	-15.218	1.00	9.33	B
ATOM	3431	CA	ILE	B	78	5.427	15.449	-16.628	1.00	9.86	B
ATOM	3432	CB	ILE	B	78	5.451	16.940	-17.049	1.00	11.48	B
ATOM	3433	CG2	ILE	B	78	6.191	17.139	-18.424	1.00	13.90	B
ATOM	3434	CG1	ILE	B	78	3.976	17.389	-17.151	1.00	13.19	B
ATOM	3435	CD1	ILE	B	78	3.776	18.939	-17.260	1.00	16.24	B
ATOM	3436	C	ILE	B	78	6.817	14.832	-16.839	1.00	9.23	B
ATOM	3437	O	ILE	B	78	6.993	13.993	-17.726	1.00	10.91	B
ATOM	3438	N	CYS	B	79	7.762	15.226	-16.013	1.00	10.15	B
ATOM	3439	CA	CYS	B	79	9.131	14.699	-16.223	1.00	10.57	B
ATOM	3440	CB	CYS	B	79	10.081	15.403	-15.269	1.00	10.45	B
ATOM	3441	SG	CYS	B	79	10.273	17.176	-15.649	1.00	15.50	B
ATOM	3442	C	CYS	B	79	9.176	13.190	-16.024	1.00	12.39	B
ATOM	3443	O	CYS	B	79	9.819	12.455	-16.788	1.00	13.55	B
ATOM	3444	N	ARG	B	80	8.500	12.725	-14.986	1.00	10.64	B
ATOM	3445	CA	ARG	B	80	8.491	11.273	-14.719	1.00	12.98	B
ATOM	3446	CB	ARG	B	80	7.744	11.007	-13.399	1.00	15.52	B
ATOM	3447	C	ARG	B	80	7.791	9.534	-12.911	1.00	20.13	B
ATOM	3448	O	ARG	B	80	6.843	9.325	-11.713	1.00	25.38	B
ATOM	3449	NE	ARG	B	80	5.482	9.714	-12.093	1.00	31.58	B
ATOM	3450	CZ	ARG	B	80	4.456	9.888	-11.254	1.00	33.35	B
ATOM	3451	NH1	ARG	B	80	4.598	9.704	-9.939	1.00	35.49	B
ATOM	3452	NH2	ARG	B	80	3.280	10.257	-11.732	1.00	34.33	B
ATOM	3453	C	ARG	B	80	7.819	10.507	-15.846	1.00	13.18	B
ATOM	3454	O	ARG	B	80	8.159	9.360	-16.140	1.00	13.55	B
ATOM	3455	N	GLY	B	81	6.836	11.128	-16.484	1.00	11.84	B
ATOM	3456	CA	GLY	B	81	6.116	10.437	-17.522	1.00	11.90	B
ATOM	3457	C	GLY	B	81	6.781	10.356	-18.869	1.00	11.01	B
ATOM	3458	O	GLY	B	81	6.335	9.605	-19.734	1.00	11.50	B
ATOM	3459	N	LEU	B	82	7.806	11.188	-19.071	1.00	11.31	B
ATOM	3460	CA	LEU	B	82	8.514	11.169	-20.328	1.00	9.84	B
ATOM	3461	CB	LEU	B	82	9.370	12.430	-20.446	1.00	8.66	B
ATOM	3462	CG	LEU	B	82	8.522	13.680	-20.801	1.00	9.38	B
ATOM	3463	CD1	LEU	B	82	9.372	14.967	-20.574	1.00	9.37	B
ATOM	3464	CD2	LEU	B	82	8.050	13.551	-22.262	1.00	11.14	B
ATOM	3465	C	LEU	B	82	9.376	9.916	-20.380	1.00	11.17	B

Figure 1 (continued 35)

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ATOM	3466	O	LEU	B	82	9.726	9.344	-19.347	1.00	12.58	B
ATOM	3467	N	PRO	B	83	9.758	9.523	-21.590	1.00	11.69	B
ATOM	3468	CD	PRO	B	83	9.531	10.208	-22.863	1.00	13.36	B
ATOM	3469	CA	PRO	B	83	10.575	8.309	-21.770	1.00	12.94	B
ATOM	3470	C	PRO	B	83	10.597	8.140	-23.290	1.00	15.08	B
ATOM	3471	CG	PRO	B	83	10.505	9.493	-23.806	1.00	14.86	B
ATOM	3472	C	PRO	B	83	11.964	8.393	-21.150	1.00	15.17	B
ATOM	3473	O	PRO	B	83	12.542	9.473	-21.023	1.00	14.86	B
ATOM	3474	N	GLU	B	84	12.495	7.237	-20.759	1.00	15.45	B
ATOM	3475	CA	GLU	B	84	13.817	7.220	-20.152	1.00	15.30	B
ATOM	3476	CB	GLU	B	84	14.193	5.761	-19.825	1.00	17.19	B
ATOM	3477	CG	GLU	B	84	15.507	5.588	-19.128	1.00	20.25	B
ATOM	3478	CD	GLU	B	84	15.564	4.266	-18.419	1.00	22.78	B
ATOM	3479	OE1	GLU	B	84	14.981	3.297	-18.955	1.00	27.86	B
ATOM	3480	OE2	GLU	B	84	16.180	4.197	-17.344	1.00	25.77	B
ATOM	3481	C	GLU	B	84	14.831	7.848	-21.116	1.00	13.55	B
ATOM	3482	O	GLU	B	84	14.815	7.576	-22.325	1.00	16.08	B
ATOM	3483	N	GLY	B	85	15.682	8.719	-20.573	1.00	15.12	B
ATOM	3484	CA	GLY	B	85	16.714	9.359	-21.386	1.00	15.70	B
ATOM	3485	C	GLY	B	85	16.279	10.612	-22.136	1.00	16.21	B
ATOM	3486	O	GLY	B	85	17.088	11.268	-22.797	1.00	17.94	B
ATOM	3487	N	ALA	B	86	14.995	10.955	-22.013	1.00	13.60	B
ATOM	3488	CA	ALA	B	86	14.450	12.128	-22.688	1.00	13.37	B
ATOM	3489	CB	ALA	B	86	12.944	12.293	-22.330	1.00	15.70	B
ATOM	3490	C	ALA	B	86	15.161	13.416	-22.324	1.00	12.98	B
ATOM	3491	O	ALA	B	86	15.551	13.631	-21.183	1.00	13.52	B
ATOM	3492	N	GLU	B	87	15.341	14.285	-23.316	1.00	12.60	B
ATOM	3493	CA	GLU	B	87	15.926	15.594	-23.086	1.00	12.20	B
ATOM	3494	CB	GLU	B	87	16.650	16.050	-24.339	1.00	16.46	B
ATOM	3495	CG	GLU	B	87	17.818	15.137	-24.688	1.00	20.50	B
ATOM	3496	CD	GLU	B	87	18.945	15.208	-23.669	1.00	24.25	B
ATOM	3497	OE1	GLU	B	87	18.958	16.145	-22.844	1.00	21.60	B
ATOM	3498	OE2	GLU	B	87	19.827	14.308	-23.718	1.00	25.73	B
ATOM	3499	C	GLU	B	87	14.734	16.512	-22.814	1.00	12.64	B
ATOM	3500	O	GLU	B	87	13.810	16.527	-23.623	1.00	15.78	B
ATOM	3501	N	ILE	B	88	14.770	17.241	-21.707	1.00	12.08	B
ATOM	3502	CA	ILE	B	88	13.645	18.127	-21.325	1.00	11.17	B
ATOM	3503	CB	ILE	B	88	13.218	17.788	-19.878	1.00	11.48	B
ATOM	3504	CG2	ILE	B	88	11.990	18.637	-19.452	1.00	12.56	B
ATOM	3505	CG1	ILE	B	88	12.887	16.294	-19.815	1.00	12.51	B
ATOM	3506	CD1	ILE	B	88	12.482	15.794	-18.471	1.00	11.91	B
ATOM	3507	C	ILE	B	88	14.067	19.573	-21.468	1.00	10.83	B
ATOM	3508	O	ILE	B	88	14.909	20.066	-20.691	1.00	12.26	B
ATOM	3509	N	ALA	B	89	13.477	20.261	-22.448	1.00	10.23	B
ATOM	3510	CA	ALA	B	89	13.802	21.659	-22.723	1.00	10.42	B
ATOM	3511	CB	ALA	B	89	13.784	21.911	-24.227	1.00	11.36	B
ATOM	3512	C	ALA	B	89	12.738	22.517	-22.046	1.00	11.07	B
ATOM	3513	O	ALA	B	89	11.542	22.297	-22.226	1.00	13.01	B
ATOM	3514	N	VAL	B	90	13.196	23.508	-21.307	1.00	10.02	B
ATOM	3515	CA	VAL	B	90	12.301	24.367	-20.549	1.00	9.76	B
ATOM	3516	CB	VAL	B	90	12.499	24.064	-19.045	1.00	10.85	B
ATOM	3517	CG1	VAL	B	90	11.583	24.955	-18.217	1.00	12.19	B
ATOM	3518	CG2	VAL	B	90	12.171	22.613	-18.750	1.00	11.27	B
ATOM	3519	C	VAL	B	90	12.577	25.830	-20.791	1.00	11.53	B
ATOM	3520	O	VAL	B	90	13.731	26.256	-20.768	1.00	13.48	B
ATOM	3521	N	GLN	B	91	11.523	26.617	-21.015	1.00	11.55	B
ATOM	3522	CA	GLN	B	91	11.705	28.051	-21.210	1.00	14.62	B
ATOM	3523	CB	GLN	B	91	11.889	28.401	-22.692	1.00	18.48	B
ATOM	3524	CG	GLN	B	91	12.135	29.913	-22.891	1.00	26.33	B
ATOM	3525	CD	GLN	B	91	12.980	30.211	-24.112	1.00	29.12	B
ATOM	3526	OE1	GLN	B	91	13.538	31.308	-24.238	1.00	34.56	B
ATOM	3527	NE2	GLN	B	91	13.073	29.248	-25.024	1.00	31.87	B
ATOM	3528	C	GLN	B	91	10.550	28.838	-20.631	1.00	14.08	B
ATOM	3529	O	GLN	B	91	9.367	28.487	-20.811	1.00	13.76	B
ATOM	3530	N	LEU	B	92	10.908	29.885	-19.884	1.00	14.73	B
ATOM	3531	CA	LEU	B	92	9.928	30.771	-19.267	1.00	15.30	B
ATOM	3532	CB	LEU	B	92	10.575	31.606	-18.144	1.00	16.00	B
ATOM	3533	CG	LEU	B	92	9.626	32.613	-17.459	1.00	15.51	B
ATOM	3534	CD1	LEU	B	92	8.460	31.882	-16.765	1.00	18.05	B
ATOM	3535	CD2	LEU	B	92	10.387	33.405	-16.426	1.00	17.67	B
ATOM	3536	C	LEU	B	92	9.435	31.694	-20.368	1.00	16.50	B
ATOM	3537	O	LEU	B	92	10.259	32.293	-21.102	1.00	17.36	B
ATOM	3538	N	GLU	B	93	8.107	31.790	-20.487	1.00	17.70	B
ATOM	3539	CA	GLU	B	93	7.456	32.645	-21.469	1.00	20.10	B
ATOM	3540	CB	GLU	B	93	6.889	31.788	-22.615	1.00	19.07	B
ATOM	3541	CD	GLU	B	93	8.021	30.998	-23.341	1.00	20.16	B
ATOM	3542	OE1	GLU	B	93	7.622	30.371	-24.678	1.00	21.44	B
ATOM	3543	OE2	GLU	B	93	6.413	30.147	-24.893	1.00	22.08	B
ATOM	3544	C	GLU	B	93	8.530	30.087	-25.504	1.00	20.59	B
ATOM	3545	O	GLU	B	93	6.358	33.451	-20.767	1.00	21.41	B
ATOM	3546	N	GLY	B	94	5.165	33.286	-21.039	1.00	22.54	B
ATOM	3547	CA	GLY	B	94	6.774	34.296	-19.821	1.00	23.49	B
ATOM	3548	C	GLY	B	94	5.826	35.136	-19.099	1.00	23.13	B
ATOM	3549	O	GLY	B	94	4.835	34.435	-18.182	1.00	23.80	B
ATOM	3550	N	GLU	B	95	5.205	33.923	-17.126	1.00	23.56	B
ATOM	3551	CA	GLU	B	95	3.569	34.428	-18.574	1.00	21.90	B
ATOM	3552	CB	GLU	B	95	2.539	33.797	-17.756	1.00	22.03	B
ATOM	3553	CG	GLU	B	95	1.135	34.201	-18.269	1.00	25.70	B
ATOM	3554	CD	GLU	B	95	0.715	33.489	-19.565	1.00	32.06	B
ATOM	3555	OE1	GLU	B	95	-0.577	34.015	-20.188	1.00	34.90	B
ATOM	3556	OE2	GLU	B	95	-1.491	34.428	-19.437	1.00	35.44	B
ATOM	3557	C	GLU	B	95	-0.679	33.994	-21.442	1.00	37.09	B
ATOM	3558	O	GLU	B	95	2.680	32.262	-17.760	1.00	20.12	B
ATOM	3559	N	GLU	B	95	2.076	31.573	-16.932	1.00	19.55	B
ATOM	3560	CA	ARG	B	96	3.465	31.726	-18.694	1.00	17.37	B
ATOM	3561	CB	ARG	B	96	3.605	30.271	-18.751	1.00	14.55	B
ATOM	3562	CG	ARG	B	96	2.777	29.683	-19.912	1.00	16.86	B
ATOM	3563	CD	ARG	B	96	3.296	29.392	-21.341	1.00	16.89	B
ATOM	3564	OE1	ARG	B	96	4.258	28.903	-21.876	1.00	20.34	B
ATOM	3565	NE	ARG	B	96	4.551	28.994	-23.319	1.00	22.54	B

Figure 1 (continued 36)

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ATOM	3566	CZ	ARG	B	96	3.842	28.445	-24.308	1.00	25.11	B
ATOM	3567	NH1	ARG	B	96	2.742	27.746	-24.054	1.00	24.38	B
ATOM	3568	NH2	ARG	B	96	4.276	28.546	-25.577	1.00	20.68	B
ATOM	3569	C	ARG	B	96	5.025	29.829	-19.904	1.00	13.94	B
ATOM	3570	O	ARG	B	96	5.883	30.602	-19.321	1.00	14.85	B
ATOM	3571	N	MET	B	97	5.266	28.578	-18.520	1.00	12.30	B
ATOM	3572	CA	MET	B	97	6.582	27.961	-18.667	1.00	10.91	B
ATOM	3573	CG	MET	B	97	7.093	27.392	-17.326	1.00	10.86	B
ATOM	3574	CG	MET	B	97	8.503	26.885	-17.487	1.00	14.36	B
ATOM	3575	SD	MET	B	97	9.268	26.288	-15.952	1.00	14.09	B
ATOM	3576	CE	MET	B	97	8.674	24.617	-15.920	1.00	15.27	B
ATOM	3577	C	MET	B	97	6.336	26.817	-19.641	1.00	11.29	B
ATOM	3578	O	MET	B	97	5.493	25.956	-19.386	1.00	11.55	B
ATOM	3579	N	LEU	B	98	7.099	26.798	-20.750	1.00	10.37	B
ATOM	3580	CA	LEU	B	98	6.935	25.818	-21.793	1.00	9.09	B
ATOM	3581	CB	LEU	B	98	7.140	26.502	-23.145	1.00	10.04	B
ATOM	3582	CG	LEU	B	98	7.119	25.556	-24.343	1.00	13.03	B
ATOM	3583	CD1	LEU	B	98	5.756	24.875	-24.484	1.00	14.58	B
ATOM	3584	CD2	LEU	B	98	7.499	26.390	-25.593	1.00	15.51	B
ATOM	3585	C	LEU	B	98	7.936	24.703	-21.615	1.00	10.17	B
ATOM	3586	O	LEU	B	98	9.121	24.991	-21.439	1.00	12.00	B
ATOM	3587	N	VAL	B	99	7.440	23.469	-21.569	1.00	8.14	B
ATOM	3588	CA	VAL	B	99	8.303	22.284	-21.423	1.00	9.99	B
ATOM	3589	CB	VAL	B	99	7.831	21.408	-20.182	1.00	8.49	B
ATOM	3590	CG1	VAL	B	99	8.712	20.156	-20.085	1.00	12.22	B
ATOM	3591	CG2	VAL	B	99	7.813	22.225	-18.916	1.00	10.21	B
ATOM	3592	C	VAL	B	99	8.169	21.454	-22.700	1.00	11.04	B
ATOM	3593	O	VAL	B	99	7.031	21.087	-23.108	1.00	10.88	B
ATOM	3594	N	ARG	B	100	9.293	21.137	-23.366	1.00	8.40	B
ATOM	3595	CA	ARG	B	100	9.218	20.363	-24.593	1.00	8.30	B
ATOM	3596	CB	ARG	B	100	9.613	21.220	-25.829	1.00	10.50	B
ATOM	3597	CG	ARG	B	100	8.754	22.464	-26.057	1.00	11.28	B
ATOM	3598	CD	ARG	B	100	9.404	23.363	-27.152	1.00	15.41	B
ATOM	3599	NE	ARG	B	100	10.676	23.920	-26.707	1.00	16.70	B
ATOM	3600	CZ	ARG	B	100	11.829	23.803	-27.375	1.00	17.28	B
ATOM	3601	NH1	ARG	B	100	11.889	23.144	-28.526	1.00	21.89	B
ATOM	3602	NH2	ARG	B	100	12.927	24.341	-26.876	1.00	22.39	B
ATOM	3603	C	ARG	B	100	10.176	19.198	-24.523	1.00	9.77	B
ATOM	3604	O	ARG	B	100	11.283	19.325	-23.982	1.00	9.86	B
ATOM	3605	N	SER	B	101	9.725	18.074	-25.051	1.00	7.91	B
ATOM	3606	CA	SER	B	101	10.578	16.881	-25.125	1.00	10.45	B
ATOM	3607	CB	SER	B	101	10.549	16.126	-23.787	1.00	10.43	B
ATOM	3608	OG	SER	B	101	11.462	14.998	-23.840	1.00	13.17	B
ATOM	3609	C	SER	B	101	10.043	16.057	-26.265	1.00	12.22	B
ATOM	3610	O	SER	B	101	8.875	15.686	-26.263	1.00	11.21	B
ATOM	3611	N	GLY	B	102	10.900	15.720	-27.235	1.00	11.77	B
ATOM	3612	CA	GLY	B	102	10.396	14.967	-28.376	1.00	11.79	B
ATOM	3613	C	GLY	B	102	9.269	15.772	-29.010	1.00	11.95	B
ATOM	3614	O	GLY	B	102	9.440	16.944	-29.277	1.00	13.86	B
ATOM	3615	N	ARG	B	103	8.113	15.137	-29.248	1.00	13.24	B
ATOM	3616	CA	ARG	B	103	6.950	15.842	-29.786	1.00	13.56	B
ATOM	3617	CB	ARG	B	103	6.404	15.140	-31.024	1.00	15.71	B
ATOM	3618	CG	ARG	B	103	7.403	15.240	-32.172	1.00	18.07	B
ATOM	3619	CD	ARG	B	103	6.753	14.857	-33.491	1.00	20.42	B
ATOM	3620	NE	ARG	B	103	6.426	13.446	-33.518	1.00	21.82	B
ATOM	3621	CZ	ARG	B	103	5.798	12.861	-34.539	1.00	24.65	B
ATOM	3622	NH1	ARG	B	103	5.437	13.580	-35.598	1.00	24.54	B
ATOM	3623	NH2	ARG	B	103	5.564	11.560	-34.517	1.00	25.63	B
ATOM	3624	C	ARG	B	103	5.893	15.933	-28.697	1.00	13.10	B
ATOM	3625	O	ARG	B	103	4.685	15.809	-28.966	1.00	14.85	B
ATOM	3626	N	SER	B	104	6.372	16.100	-27.468	1.00	10.09	B
ATOM	3627	CA	SER	B	104	5.503	16.309	-26.293	1.00	11.86	B
ATOM	3628	CB	SER	B	104	5.888	15.378	-25.138	1.00	12.18	B
ATOM	3629	OG	SER	B	104	5.938	14.020	-25.597	1.00	12.05	B
ATOM	3630	C	SER	B	104	5.701	17.775	-25.877	1.00	12.30	B
ATOM	3631	O	SER	B	104	6.849	18.298	-25.815	1.00	12.26	B
ATOM	3632	N	ARG	B	105	4.689	18.470	-25.625	1.00	10.81	B
ATOM	3633	CA	ARG	B	105	4.158	19.867	-25.234	1.00	10.24	B
ATOM	3634	CB	ARG	B	105	5.004	20.772	-26.370	1.00	12.01	B
ATOM	3635	CG	ARG	B	105	4.285	20.788	-27.618	1.00	12.34	B
ATOM	3636	CD	ARG	B	105	4.285	21.560	-28.760	1.00	13.57	B
ATOM	3637	NE	ARG	B	105	3.799	22.896	-28.364	1.00	13.32	B
ATOM	3638	CZ	ARG	B	105	4.552	23.991	-28.366	1.00	14.90	B
ATOM	3639	NH1	ARG	B	105	5.822	23.903	-28.740	1.00	13.50	B
ATOM	3640	NH2	ARG	B	105	4.037	25.165	-28.014	1.00	14.92	B
ATOM	3641	C	ARG	B	105	3.757	20.122	-24.052	1.00	9.77	B
ATOM	3642	O	ARG	B	105	2.639	19.588	-24.006	1.00	11.33	B
ATOM	3643	N	SER	B	106	4.221	20.929	-23.108	1.00	10.77	B
ATOM	3644	CA	PHE	B	106	3.380	21.252	-21.939	1.00	9.20	B
ATOM	3645	CB	PHE	B	106	3.795	20.410	-20.719	1.00	10.28	B
ATOM	3646	CG	PHE	B	106	3.876	18.955	-21.000	1.00	9.68	B
ATOM	3647	CD1	PHE	B	106	5.019	18.433	-21.591	1.00	12.41	B
ATOM	3648	CD2	PHE	B	106	2.775	18.115	-20.793	1.00	12.06	B
ATOM	3649	CE1	PHE	B	106	5.072	17.120	-21.982	1.00	12.35	B
ATOM	3650	CE2	PHE	B	106	2.812	16.797	-21.182	1.00	13.89	B
ATOM	3651	C	PHE	B	106	3.953	16.280	-21.783	1.00	14.71	B
ATOM	3652	O	PHE	B	106	3.525	22.714	-21.579	1.00	12.00	B
ATOM	3653	N	PHE	B	106	4.649	23.241	-21.528	1.00	11.63	B
ATOM	3654	CA	SER	B	107	2.389	23.375	-21.291	1.00	10.03	B
ATOM	3655	CB	SER	B	107	2.415	24.766	-20.896	1.00	13.00	B
ATOM	3656	CG	SER	B	107	1.559	25.595	-21.848	1.00	13.92	B
ATOM	3657	OG	SER	B	107	1.547	26.962	-21.475	1.00	17.21	B
ATOM	3658	C	SER	B	107	1.897	24.858	-19.471	1.00	13.30	B
ATOM	3659	O	SER	B	107	0.741	24.542	-19.219	1.00	13.25	B
ATOM	3660	N	LEU	B	108	2.774	25.213	-18.543	1.00	11.97	B
ATOM	3661	CA	LEU	B	108	2.399	25.325	-17.130	1.00	12.30	B
ATOM	3662	CB	LEU	B	108	3.497	24.741	-16.221	1.00	13.26	B
ATOM	3663	CG	LEU	B	108	3.715	23.249	-16.427	1.00	15.24	B
ATOM	3664	CD1	LEU	B	108	4.883	22.751	-15.567	1.00	14.96	B
ATOM	3665	CD2	LEU	B	108	2.441	22.561	-16.079	1.00	15.65	B

Figure 1 (continued 37)

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ATOM	3666	C	LEU	B	108	2.210	26.768	-15.703	1.00	12.13	B
ATOM	3667	O	LEU	B	108	2.936	27.647	-17.149	1.00	12.73	B
ATOM	3668	N	SER	B	109	1.249	27.021	-15.807	1.00	13.50	B
ATOM	3669	CEA	SER	B	109	1.036	28.382	-15.313	1.00	15.61	B
ATOM	3670	CGA	SER	B	109	-0.345	28.465	-14.642	1.00	17.76	B
ATOM	3671	CGC	SER	B	109	-0.427	27.508	-13.599	1.00	25.01	B
ATOM	3672	CC	SER	B	109	2.118	28.695	-14.290	1.00	15.85	B
ATOM	3673	O	SER	B	109	2.547	27.799	-13.536	1.00	18.85	B
ATOM	3674	N	THR	B	110	2.550	28.935	-14.259	1.00	13.95	B
ATOM	3675	CEA	THR	B	110	3.587	30.367	-13.332	1.00	14.07	B
ATOM	3676	CEB	THR	B	110	4.749	31.074	-14.088	1.00	15.61	B
ATOM	3677	CG1	THR	B	110	4.262	32.260	-14.719	1.00	15.22	B
ATOM	3678	CG2	THR	B	110	5.333	30.173	-15.168	1.00	13.87	B
ATOM	3679	O	THR	B	110	3.081	31.376	-12.323	1.00	14.62	B
ATOM	3680	N	THR	B	110	2.028	32.023	-12.521	1.00	16.48	B
ATOM	3681	N	LEU	B	111	3.835	31.498	-11.234	1.00	14.53	B
ATOM	3682	CGA	LEU	B	111	3.626	32.540	-10.236	1.00	14.82	B
ATOM	3683	CGB	LEU	B	111	3.048	31.999	-8.916	1.00	15.27	B
ATOM	3684	CGC	LEU	B	111	1.577	31.535	-8.991	1.00	16.13	B
ATOM	3685	CGD1	LEU	B	111	1.177	30.854	-7.706	1.00	15.76	B
ATOM	3686	CGD2	LEU	B	111	0.650	32.769	-9.243	1.00	15.24	B
ATOM	3687	O	LEU	B	111	5.047	33.114	-10.070	1.00	16.26	B
ATOM	3688	N	LEU	B	111	6.064	32.403	-10.174	1.00	16.00	B
ATOM	3689	CEA	PRO	B	112	5.158	34.428	-9.873	1.00	15.54	B
ATOM	3690	CEB	PRO	B	112	4.031	35.374	-9.725	1.00	18.98	B
ATOM	3691	CGA	PRO	B	112	6.430	35.129	-9.711	1.00	16.92	B
ATOM	3692	CGB	PRO	B	112	5.984	36.546	-9.325	1.00	17.38	B
ATOM	3693	CGC	PRO	B	112	4.697	36.676	-10.033	1.00	19.99	B
ATOM	3694	CGD	PRO	B	112	7.388	34.571	-8.674	1.00	15.89	B
ATOM	3695	O	PRO	B	112	6.978	34.259	-7.552	1.00	17.87	B
ATOM	3696	N	ALA	B	113	8.654	34.451	-9.066	1.00	17.65	B
ATOM	3697	CEA	ALA	B	113	9.702	33.993	-8.159	1.00	17.75	B
ATOM	3698	CEB	ALA	B	113	11.050	33.908	-8.901	1.00	18.59	B
ATOM	3699	CGA	ALA	B	113	9.794	35.003	-6.997	1.00	19.95	B
ATOM	3700	CGB	ALA	B	113	10.098	34.604	-5.873	1.00	18.56	B
ATOM	3701	CGC	ALA	B	114	9.494	36.285	-7.254	1.00	19.88	B
ATOM	3702	CGD	ALA	B	114	9.546	37.297	-6.190	1.00	22.97	B
ATOM	3703	O	ALA	B	114	9.274	38.686	-6.762	1.00	24.68	B
ATOM	3704	N	ALA	B	114	8.551	37.025	-5.073	1.00	24.13	B
ATOM	3705	CEA	ALA	B	114	8.735	37.506	-3.948	1.00	25.27	B
ATOM	3706	CEB	ASP	B	115	7.499	36.270	-5.374	1.00	22.97	B
ATOM	3707	CGA	ASP	B	115	6.458	35.936	-4.398	1.00	21.92	B
ATOM	3708	CGB	ASP	B	115	5.095	35.838	-5.085	1.00	25.25	B
ATOM	3709	CGC	ASP	B	115	4.653	37.144	-5.702	1.00	27.35	B
ATOM	3710	CGD1	ASP	B	115	5.197	38.200	-5.325	1.00	32.10	B
ATOM	3711	CGD2	ASP	B	115	3.756	37.115	-6.562	1.00	30.15	B
ATOM	3712	O	ASP	B	115	6.686	34.620	-3.639	1.00	20.39	B
ATOM	3713	N	ASP	B	115	5.892	34.256	-2.770	1.00	19.74	B
ATOM	3714	CEA	PHE	B	116	7.743	33.883	-3.987	1.00	17.71	B
ATOM	3715	CEB	PHE	B	116	7.987	32.602	-3.323	1.00	18.38	B
ATOM	3716	CGA	PHE	B	116	9.004	31.796	-4.157	1.00	17.21	B
ATOM	3717	CGB	PHE	B	116	9.043	30.332	-3.810	1.00	18.03	B
ATOM	3718	CGC	PHE	B	116	8.071	29.452	-4.300	1.00	16.40	B
ATOM	3719	CGD1	PHE	B	116	10.026	29.837	-2.955	1.00	17.20	B
ATOM	3720	CGD2	PHE	B	116	8.072	28.104	-3.949	1.00	18.94	B
ATOM	3721	O	PHE	B	116	10.029	28.479	-2.596	1.00	15.80	B
ATOM	3722	N	PHE	B	116	9.057	27.613	-3.091	1.00	18.24	B
ATOM	3723	CEA	PHE	B	116	8.510	32.836	-1.896	1.00	18.89	B
ATOM	3724	CEB	PHE	B	116	9.449	33.594	-1.716	1.00	19.05	B
ATOM	3725	CGA	PRO	B	117	7.914	32.172	-0.888	1.00	20.37	B
ATOM	3726	CGB	PRO	B	117	6.913	31.117	-1.080	1.00	20.82	B
ATOM	3727	CGC	PRO	B	117	8.284	32.285	0.535	1.00	22.94	B
ATOM	3728	CGD	PRO	B	117	7.397	31.244	1.226	1.00	24.98	B
ATOM	3729	O	PRO	B	117	6.285	30.991	0.290	1.00	22.83	B
ATOM	3730	N	PRO	B	117	9.736	31.922	0.684	1.00	25.37	B
ATOM	3731	CEA	PRO	B	117	10.204	31.012	0.018	1.00	26.02	B
ATOM	3732	CEB	ASN	B	118	10.441	32.630	1.556	1.00	27.41	B
ATOM	3733	CGA	ASN	B	118	11.857	32.398	1.767	1.00	30.63	B
ATOM	3734	CGB	ASN	B	118	12.638	33.537	1.081	1.00	34.20	B
ATOM	3735	CGC	ASN	B	118	14.111	33.525	1.411	1.00	36.43	B
ATOM	3736	CGD1	ASN	B	118	14.518	33.929	2.500	1.00	39.71	B
ATOM	3737	CGD2	ASN	B	118	14.922	33.052	0.472	1.00	40.26	B
ATOM	3738	O	ASN	B	118	12.103	32.399	3.275	1.00	31.98	B
ATOM	3739	N	ASN	B	118	11.683	33.332	3.959	1.00	32.47	B
ATOM	3740	CEA	LEU	B	119	12.746	31.365	3.810	1.00	31.29	B
ATOM	3741	CEB	LEU	B	119	13.013	31.372	5.713	1.00	32.34	B
ATOM	3742	CGA	LEU	B	119	13.616	30.042	5.242	1.00	32.40	B
ATOM	3743	CGB	LEU	B	119	12.712	28.820	5.889	1.00	32.42	B
ATOM	3744	CGC	LEU	B	119	13.507	27.710	6.551	1.00	34.29	B
ATOM	3745	CGD1	LEU	B	119	11.516	29.170	6.758	1.00	30.06	B
ATOM	3746	CGD2	LEU	B	119	13.996	32.502	5.540	1.00	32.87	B
ATOM	3747	O	LEU	B	119	14.922	32.751	4.767	1.00	32.78	B
ATOM	3748	N	ASP	B	120	13.785	33.170	6.668	1.00	33.27	B
ATOM	3749	CEA	ASP	B	120	14.634	34.264	7.106	1.00	35.53	B
ATOM	3750	CEB	ASP	B	120	14.100	34.820	8.442	1.00	38.51	B
ATOM	3751	CGA	ASP	B	120	14.813	36.102	8.896	1.00	41.15	B
ATOM	3752	CGB	ASP	B	120	15.288	36.880	8.032	1.00	42.97	B
ATOM	3753	CGC	ASP	B	120	14.878	36.341	10.128	1.00	41.78	B
ATOM	3754	CGD1	ASP	B	120	16.076	33.793	7.240	1.00	34.92	B
ATOM	3755	CGD2	ASP	B	120	16.366	32.615	7.430	1.00	33.81	B
ATOM	3756	O	ASP	B	121	16.984	34.737	7.103	1.00	34.47	B
ATOM	3757	N	ASP	B	121	18.393	34.466	7.212	1.00	33.96	B
ATOM	3758	CEA	ASP	B	121	19.125	35.724	6.770	1.00	38.12	B
ATOM	3759	CEB	ASP	B	121	18.471	36.339	5.540	1.00	41.54	B
ATOM	3760	CGA	ASP	B	121	18.665	35.786	4.433	1.00	42.91	B
ATOM	3761	CGB	ASP	B	121	17.730	37.344	5.687	1.00	44.40	B
ATOM	3762	CGC	ASP	B	121	18.648	34.144	8.672	1.00	31.06	B
ATOM	3763	CGD	ASP	B	121	17.935	34.611	9.549	1.00	30.33	B
ATOM	3764	O	TRP	B	122	19.642	33.314	8.927	1.00	29.45	B
ATOM	3765	N	TRP	B	122	19.953	32.969	10.301	1.00	26.54	B

Figure 1 (continued 38)

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ATOM	3766	CB	TRP	B	122	19.021	31.833	10.766	1.00	24.27	B
ATOM	3767	CG	TRP	B	122	19.072	30.629	9.899	1.00	23.67	B
ATOM	3768	CD2	TRP	B	122	19.832	29.445	10.127	1.00	23.03	B
ATOM	3769	CE2	TRP	B	122	19.617	28.587	9.027	1.00	24.46	B
ATOM	3770	CE3	TRP	B	122	20.680	29.020	11.157	1.00	21.61	B
ATOM	3771	CD1	TRP	B	122	18.435	30.451	8.697	1.00	25.67	B
ATOM	3772	NE1	TRP	B	122	18.760	29.225	8.167	1.00	25.03	B
ATOM	3773	CZ2	TRP	B	122	20.224	27.327	8.929	1.00	24.86	B
ATOM	3774	CZ3	TRP	B	122	21.276	27.769	11.061	1.00	21.60	B
ATOM	3775	CH2	TRP	B	122	21.047	26.940	9.956	1.00	25.02	B
ATOM	3776	C	TRP	B	122	21.416	32.581	10.381	1.00	25.76	B
ATOM	3777	O	TRP	B	122	22.081	32.419	9.354	1.00	25.40	B
ATOM	3778	N	GLN	B	123	21.932	32.437	11.600	1.00	22.86	B
ATOM	3779	CA	GLN	B	123	23.330	32.106	11.786	1.00	25.29	B
ATOM	3780	CB	GLN	B	123	23.960	33.225	12.614	1.00	23.33	B
ATOM	3781	CG	GLN	B	123	23.736	34.611	12.017	1.00	28.45	B
ATOM	3782	CD	GLN	B	123	24.576	34.837	10.772	1.00	28.70	B
ATOM	3783	OE1	GLN	B	123	24.445	35.856	10.099	1.00	32.60	B
ATOM	3784	NE2	GLN	B	123	25.447	33.889	10.469	1.00	32.57	B
ATOM	3785	C	GLN	B	123	23.537	30.762	12.492	1.00	24.00	B
ATOM	3786	O	GLN	B	123	22.879	30.502	13.494	1.00	25.77	B
ATOM	3787	N	SER	B	124	24.440	29.917	11.994	1.00	23.58	B
ATOM	3788	CA	SER	B	124	24.680	28.643	12.680	1.00	24.40	B
ATOM	3789	CB	SER	B	124	25.295	27.574	11.778	1.00	26.13	B
ATOM	3790	OG	SER	B	124	26.636	27.883	11.441	1.00	32.13	B
ATOM	3791	C	SER	B	124	25.600	28.849	13.870	1.00	24.43	B
ATOM	3792	O	SER	B	124	26.566	29.622	13.803	1.00	24.71	B
ATOM	3793	N	GLU	B	125	25.274	28.155	14.952	1.00	23.06	B
ATOM	3794	CA	GLU	B	125	26.035	28.205	16.203	1.00	24.57	B
ATOM	3795	CB	GLU	B	125	25.093	28.516	17.360	1.00	25.73	B
ATOM	3796	CG	GLU	B	125	24.399	29.857	17.254	1.00	32.47	B
ATOM	3797	CD	GLU	B	125	23.353	30.051	18.344	1.00	35.90	B
ATOM	3798	OE1	GLU	B	125	23.423	29.345	19.381	1.00	39.08	B
ATOM	3799	OE2	GLU	B	125	22.464	30.912	18.168	1.00	39.18	B
ATOM	3800	C	GLU	B	125	26.786	26.907	16.508	1.00	24.50	B
ATOM	3801	O	GLU	B	125	27.665	26.879	17.382	1.00	24.43	B
ATOM	3802	N	VAL	B	126	26.419	25.815	15.844	1.00	22.81	B
ATOM	3803	CA	VAL	B	126	27.106	24.539	16.031	1.00	24.05	B
ATOM	3804	CB	VAL	B	126	26.434	23.637	17.119	1.00	24.27	B
ATOM	3805	CG1	VAL	B	126	25.027	23.339	16.751	1.00	25.14	B
ATOM	3806	CG2	VAL	B	126	27.216	22.320	17.271	1.00	27.01	B
ATOM	3807	C	VAL	B	126	27.078	23.835	14.690	1.00	23.78	B
ATOM	3808	O	VAL	B	126	26.073	23.885	13.967	1.00	24.92	B
ATOM	3809	N	GLU	B	127	28.182	23.193	14.344	1.00	22.15	B
ATOM	3810	CA	GLU	B	127	28.281	22.509	13.081	1.00	21.91	B
ATOM	3811	CB	GLU	B	127	29.002	23.394	12.051	1.00	23.10	B
ATOM	3812	CG	GLU	B	127	28.426	24.768	11.966	1.00	26.12	B
ATOM	3813	CD	GLU	B	127	29.056	25.636	10.884	1.00	27.63	B
ATOM	3814	OE1	GLU	B	127	28.434	26.672	10.546	1.00	27.53	B
ATOM	3815	OE2	GLU	B	127	30.157	25.298	10.403	1.00	28.31	B
ATOM	3816	C	GLU	B	127	29.069	21.240	13.254	1.00	21.48	B
ATOM	3817	O	GLU	B	127	30.034	21.189	14.027	1.00	22.56	B
ATOM	3818	N	PHE	B	128	28.665	20.215	12.536	1.00	20.20	B
ATOM	3819	CA	PHE	B	128	29.377	18.956	12.576	1.00	19.84	B
ATOM	3820	CB	PHE	B	128	29.096	18.211	13.895	1.00	21.34	B
ATOM	3821	CG	PHE	B	128	27.632	18.001	14.172	1.00	19.99	B
ATOM	3822	CD1	PHE	B	128	26.892	18.969	14.829	1.00	20.54	B
ATOM	3823	CD2	PHE	B	128	26.993	16.851	13.729	1.00	19.54	B
ATOM	3824	CE1	PHE	B	128	25.516	18.802	15.043	1.00	18.79	B
ATOM	3825	CE2	PHE	B	128	25.616	16.672	13.938	1.00	20.76	B
ATOM	3826	CZ	PHE	B	128	24.886	17.646	14.591	1.00	20.20	B
ATOM	3827	C	PHE	B	128	28.997	18.096	11.392	1.00	21.44	B
ATOM	3828	O	PHE	B	128	27.986	18.338	10.707	1.00	19.41	B
ATOM	3829	N	THR	B	129	29.836	17.110	11.111	1.00	19.99	B
ATOM	3830	CA	THR	B	129	29.562	16.198	10.029	1.00	22.84	B
ATOM	3831	CB	THR	B	129	30.712	16.238	8.982	1.00	25.69	B
ATOM	3832	CG1	THR	B	129	31.949	15.897	9.626	1.00	32.56	B
ATOM	3833	CG2	THR	B	129	30.846	17.633	8.404	1.00	25.73	B
ATOM	3834	C	THR	B	129	29.415	14.792	10.608	1.00	24.49	B
ATOM	3835	O	THR	B	129	30.021	14.476	11.630	1.00	26.37	B
ATOM	3836	N	LEU	B	130	28.577	13.964	10.000	1.00	24.49	B
ATOM	3837	CA	LEU	B	130	28.423	12.589	10.477	1.00	24.08	B
ATOM	3838	CB	LEU	B	130	27.407	12.505	11.633	1.00	25.54	B
ATOM	3839	CG	LEU	B	130	25.900	12.579	11.337	1.00	25.32	B
ATOM	3840	CD1	LEU	B	130	25.149	12.111	12.598	1.00	24.84	B
ATOM	3841	CD2	LEU	B	130	25.477	13.989	10.960	1.00	23.86	B
ATOM	3842	C	LEU	B	130	27.965	11.707	9.327	1.00	23.70	B
ATOM	3843	O	LEU	B	130	27.413	12.191	8.343	1.00	23.84	B
ATOM	3844	N	PRO	B	131	28.197	10.389	9.425	1.00	23.64	B
ATOM	3845	CD	PRO	B	131	28.932	9.700	10.501	1.00	22.59	B
ATOM	3846	CA	PRO	B	131	27.790	9.465	8.371	1.00	22.27	B
ATOM	3847	CB	PRO	B	131	28.311	8.105	8.871	1.00	23.69	B
ATOM	3848	CG	PRO	B	131	29.456	8.479	9.793	1.00	23.88	B
ATOM	3849	O	PRO	B	131	26.273	9.459	8.237	1.00	23.45	B
ATOM	3850	N	PRO	B	131	25.555	9.578	9.239	1.00	21.35	B
ATOM	3851	O	GLN	B	132	25.778	9.341	7.013	1.00	22.22	B
ATOM	3852	CA	GLN	B	132	24.337	9.290	6.833	1.00	24.38	B
ATOM	3853	CB	GLN	B	132	23.975	9.060	5.383	1.00	27.52	B
ATOM	3854	CG	GLN	B	132	24.306	10.174	4.466	1.00	30.36	B
ATOM	3855	CD	GLN	B	132	23.834	9.867	3.061	1.00	32.41	B
ATOM	3856	OE1	GLN	B	132	22.667	9.539	2.845	1.00	34.45	B
ATOM	3857	NE2	GLN	B	132	24.736	9.964	2.100	1.00	33.22	B
ATOM	3858	C	GLN	B	132	23.737	8.134	7.642	1.00	24.58	B
ATOM	3859	O	GLN	B	132	22.646	8.253	8.187	1.00	23.73	B
ATOM	3860	N	ALA	B	133	24.446	7.005	7.692	1.00	24.46	B
ATOM	3861	CA	ALA	B	133	23.940	5.844	8.416	1.00	23.74	B
ATOM	3862	CB	ALA	B	133	24.911	4.650	8.241	1.00	25.48	B
ATOM	3863	C	ALA	B	133	23.677	6.103	9.896	1.00	22.24	B
ATOM	3864	O	ALA	B	133	22.768	5.493	10.482	1.00	23.23	B
ATOM	3865	N	THR	B	134	24.470	6.976	10.498	1.00	21.71	B

Figure 1 (continued.39)

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ATOM	3866	CA	THR	B	134	24.329	7.337	11.906	1.00	21.35	B
ATOM	3867	CB	THR	B	134	25.520	8.155	12.368	1.00	23.54	B
ATOM	3868	OG1	THR	B	134	26.705	7.376	12.169	1.00	25.66	B
ATOM	3869	CG2	THR	B	134	25.375	8.570	13.613	1.00	22.93	B
ATOM	3870	C	THR	B	134	23.077	8.161	12.063	1.00	20.95	B
ATOM	3871	O	THR	B	134	22.329	7.988	13.053	1.00	20.93	B
ATOM	3872	N	MET	B	135	22.855	9.097	11.172	1.00	19.95	B
ATOM	3873	CA	MET	B	135	21.654	9.897	11.284	1.00	20.19	B
ATOM	3874	CB	MET	B	135	21.626	10.994	10.222	1.00	20.76	B
ATOM	3875	CG	MET	B	135	20.385	11.886	10.326	1.00	22.47	B
ATOM	3876	SD	MET	B	135	20.158	12.699	11.928	1.00	25.83	B
ATOM	3877	CE	MET	B	135	21.360	14.018	11.870	1.00	26.97	B
ATOM	3878	C	MET	B	135	20.442	8.986	11.114	1.00	18.60	B
ATOM	3879	O	MET	B	135	19.453	9.134	11.831	1.00	18.63	B
ATOM	3880	N	LYS	B	136	20.487	8.053	10.169	1.00	19.85	B
ATOM	3881	CA	LYS	B	136	19.356	7.155	9.976	1.00	21.55	B
ATOM	3882	CB	LYS	B	136	19.595	6.173	8.831	1.00	24.24	B
ATOM	3883	CG	LYS	B	136	18.382	5.263	8.598	1.00	25.85	B
ATOM	3884	CD	LYS	B	136	18.333	4.703	7.182	1.00	32.16	B
ATOM	3885	CE	LYS	B	136	19.291	3.541	7.025	1.00	33.18	B
ATOM	3886	NZ	LYS	B	136	18.863	2.381	7.861	1.00	36.66	B
ATOM	3887	C	LYS	B	136	19.092	6.348	11.249	1.00	22.36	B
ATOM	3888	O	ARG	B	137	17.957	6.211	11.685	1.00	21.54	B
ATOM	3889	N	ARG	B	137	20.154	5.791	11.819	1.00	21.72	B
ATOM	3890	CA	ARG	B	137	20.004	4.998	13.037	1.00	21.93	B
ATOM	3891	CB	ARG	B	137	21.368	4.481	13.501	1.00	24.73	B
ATOM	3892	CG	ARG	B	137	21.339	3.432	14.643	1.00	28.08	B
ATOM	3893	CD	ARG	B	137	21.297	4.069	16.012	1.00	30.79	B
ATOM	3894	NE	ARG	B	137	21.609	3.129	17.104	1.00	31.38	B
ATOM	3895	CZ	ARG	B	137	20.802	2.161	17.547	1.00	31.74	B
ATOM	3896	NH1	ARG	B	137	19.604	1.962	17.003	1.00	31.80	B
ATOM	3897	NH2	ARG	B	137	21.184	1.411	18.578	1.00	29.88	B
ATOM	3898	C	ARG	B	137	19.360	5.820	14.141	1.00	20.76	B
ATOM	3899	O	ARG	B	137	18.389	5.386	14.770	1.00	21.28	B
ATOM	3900	N	LEU	B	138	19.880	7.021	14.364	1.00	19.03	B
ATOM	3901	CA	LEU	B	138	19.355	7.902	15.415	1.00	17.43	B
ATOM	3902	CB	LEU	B	138	20.123	9.223	15.421	1.00	17.77	B
ATOM	3903	CG	LEU	B	138	21.500	9.129	16.066	1.00	18.25	B
ATOM	3904	CD1	LEU	B	138	22.325	10.379	15.773	1.00	18.28	B
ATOM	3905	CD2	LEU	B	138	21.330	8.948	17.581	1.00	18.59	B
ATOM	3906	C	LEU	B	138	17.875	8.209	15.283	1.00	19.04	B
ATOM	3907	O	LEU	B	138	17.130	8.236	16.291	1.00	17.18	B
ATOM	3908	N	ILE	B	139	17.436	8.467	14.055	1.00	16.38	B
ATOM	3909	CA	ILE	B	139	16.027	8.793	13.843	1.00	16.79	B
ATOM	3910	CB	ILE	B	139	15.811	9.516	12.479	1.00	16.68	B
ATOM	3911	CG2	ILE	B	139	14.322	9.634	12.168	1.00	20.18	B
ATOM	3912	CG1	ILE	B	139	16.478	10.889	12.561	1.00	18.34	B
ATOM	3913	CD1	ILE	B	139	16.478	11.889	11.221	1.00	19.90	B
ATOM	3914	C	ILE	B	139	15.143	7.553	13.916	1.00	16.56	B
ATOM	3915	O	ILE	B	139	14.128	7.553	14.590	1.00	16.80	B
ATOM	3916	N	GLU	B	140	15.526	6.462	13.238	1.00	15.42	B
ATOM	3917	CA	GLU	B	140	14.720	5.276	13.263	1.00	16.12	B
ATOM	3918	CB	GLU	B	140	15.316	4.232	12.322	1.00	17.99	B
ATOM	3919	CG	GLU	B	140	15.176	4.640	10.858	1.00	22.86	B
ATOM	3920	CD	GLU	B	140	15.372	3.489	9.890	1.00	27.30	B
ATOM	3921	OE1	GLU	B	140	16.289	2.678	10.103	1.00	28.72	B
ATOM	3922	OE2	GLU	B	140	14.609	3.402	8.905	1.00	31.19	B
ATOM	3923	C	GLU	B	140	14.595	4.687	14.676	1.00	15.11	B
ATOM	3924	O	GLU	B	140	13.591	4.042	15.003	1.00	17.70	B
ATOM	3925	N	ALA	B	141	15.609	4.903	15.503	1.00	15.65	B
ATOM	3926	CA	ALA	B	141	15.577	4.336	16.849	1.00	15.07	B
ATOM	3927	CB	ALA	B	141	16.963	4.469	17.487	1.00	18.37	B
ATOM	3928	C	ALA	B	141	14.530	5.000	17.751	1.00	14.92	B
ATOM	3929	O	ALA	B	141	14.080	4.409	18.734	1.00	14.51	B
ATOM	3930	N	THR	B	142	14.097	6.209	17.401	1.00	13.57	B
ATOM	3931	CA	THR	B	142	13.205	6.922	18.309	1.00	17.09	B
ATOM	3932	CB	THR	B	142	13.994	8.081	18.978	1.00	17.94	B
ATOM	3933	OG1	THR	B	142	14.329	9.057	17.962	1.00	15.35	B
ATOM	3934	CG2	THR	B	142	15.336	7.553	19.627	1.00	14.63	B
ATOM	3935	C	THR	B	142	11.943	7.507	17.706	1.00	13.14	B
ATOM	3936	O	THR	B	142	11.004	7.820	18.438	1.00	13.61	B
ATOM	3937	N	GLN	B	143	11.899	7.640	16.381	1.00	15.74	B
ATOM	3938	CA	GLN	B	143	10.752	8.313	15.743	1.00	17.04	B
ATOM	3939	CB	GLN	B	143	10.937	8.285	14.215	1.00	18.95	B
ATOM	3940	CG	GLN	B	143	9.799	8.931	13.418	1.00	22.30	B
ATOM	3941	CD	GLN	B	143	10.073	8.886	11.922	1.00	23.43	B
ATOM	3942	OE1	GLN	B	143	10.552	7.873	11.411	1.00	23.11	B
ATOM	3943	NE2	GLN	B	143	9.769	9.989	11.211	1.00	15.74	B
ATOM	3944	C	GLN	B	143	9.380	7.797	16.137	1.00	17.49	B
ATOM	3945	O	GLN	B	143	8.438	8.577	16.322	1.00	15.47	B
ATOM	3946	N	PHE	B	144	9.254	6.489	16.319	1.00	15.79	B
ATOM	3947	CA	PHE	B	144	7.951	5.942	16.640	1.00	16.45	B
ATOM	3948	CB	PHE	B	144	8.009	4.408	16.623	1.00	15.61	B
ATOM	3949	CG	PHE	B	144	8.745	3.818	17.785	1.00	14.87	B
ATOM	3950	CD1	PHE	B	144	10.129	3.644	17.740	1.00	15.49	B
ATOM	3951	CD2	PHE	B	144	8.052	3.490	18.952	1.00	14.78	B
ATOM	3952	CE1	PHE	B	144	10.825	3.158	18.849	1.00	14.34	B
ATOM	3953	CE2	PHE	B	144	8.730	3.002	20.072	1.00	15.36	B
ATOM	3954	CZ	PHE	B	144	10.108	2.836	20.033	1.00	16.39	B
ATOM	3955	C	PHE	B	144	7.390	6.402	17.979	1.00	16.31	B
ATOM	3956	O	PHE	B	144	6.196	6.252	18.206	1.00	15.52	B
ATOM	3957	N	SER	B	145	8.233	6.932	18.857	1.00	15.49	B
ATOM	3958	CA	SER	B	145	7.765	7.357	20.178	1.00	19.43	B
ATOM	3959	CB	SER	B	145	8.842	7.137	21.236	1.00	19.03	B
ATOM	3960	OG	SER	B	145	9.051	5.743	21.459	1.00	17.97	B
ATOM	3961	C	SER	B	145	7.321	8.812	20.231	1.00	17.36	B
ATOM	3962	O	SER	B	145	6.983	9.307	21.325	1.00	17.94	B
ATOM	3963	N	MET	B	146	7.362	9.507	19.093	1.00	19.19	B
ATOM	3964	CA	MET	B	146	6.910	10.907	19.066	1.00	21.36	B
ATOM	3965	CB	MET	B	146	7.260	11.560	17.711	1.00		B

Figure 1 (continued 40)

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ATOM	3966	CG	MET	B	146	8.716	11.608	17.434	1.00	19.66	
ATOM	3967	SD	MET	B	146	8.961	11.941	15.674	1.00	23.93	
ATOM	3968	CE	MET	B	146	8.838	13.621	15.659	1.00	23.07	
ATOM	3969	C	MET	B	146	5.393	10.948	19.237	1.00	19.89	
ATOM	3970	O	MET	B	146	4.683	10.038	18.798	1.00	21.24	
ATOM	3971	N	ALA	B	147	4.879	12.014	19.853	1.00	21.60	
ATOM	3972	CA	ALA	B	147	3.438	12.137	20.009	1.00	24.00	
ATOM	3973	CB	ALA	B	147	3.112	13.270	21.028	1.00	23.97	
ATOM	3974	C	ALA	B	147	2.775	12.439	18.661	1.00	25.73	
ATOM	3975	O	ALA	B	147	3.433	12.878	17.714	1.00	23.85	
ATOM	3976	N	HIS	B	148	1.473	12.184	18.568	1.00	30.66	
ATOM	3977	CA	HIS	B	148	0.719	12.469	17.348	1.00	34.48	
ATOM	3978	CB	HIS	B	148	0.020	11.211	16.829	1.00	37.35	
ATOM	3979	CG	HIS	B	148	0.944	10.060	16.595	1.00	40.57	
ATOM	3980	CD2	HIS	B	148	0.913	8.786	17.053	1.00	41.90	
ATOM	3981	ND1	HIS	B	148	2.056	10.150	15.783	1.00	42.40	
ATOM	3982	CE1	HIS	B	148	2.672	8.981	15.754	1.00	42.24	
ATOM	3983	NE2	HIS	B	148	1.998	8.136	16.515	1.00	43.11	
ATOM	3984	C	HIS	B	148	-0.344	13.519	17.668	1.00	36.54	
ATOM	3985	O	HIS	B	148	-1.386	13.201	18.262	1.00	36.38	
ATOM	3986	N	GLN	B	149	-0.078	14.761	17.281	1.00	37.77	
ATOM	3987	CA	GLN	B	149	-1.019	15.853	17.523	1.00	39.65	
ATOM	3988	CB	GLN	B	149	-2.290	15.638	16.680	1.00	41.57	
ATOM	3989	CG	GLN	B	149	-2.022	15.462	15.185	1.00	44.91	
ATOM	3990	CD	GLN	B	149	-3.278	15.215	14.355	1.00	46.65	
ATOM	3991	OE1	GLN	B	149	-4.068	14.320	14.648	1.00	48.28	
ATOM	3992	NE2	GLN	B	149	-3.453	16.003	13.300	1.00	48.05	
ATOM	3993	C	GLN	B	149	-1.376	15.995	19.005	1.00	39.02	
ATOM	3994	O	GLN	B	149	-2.558	16.067	19.370	1.00	40.48	
ATOM	3995	N	ASP	B	150	-0.354	16.029	19.857	1.00	38.46	
ATOM	3996	CA	ASP	B	150	-0.534	16.192	21.299	1.00	37.30	
ATOM	3997	CB	ASP	B	150	0.679	15.640	22.059	1.00	37.60	
ATOM	3998	CG	ASP	B	150	0.445	15.547	23.561	1.00	38.25	
ATOM	3999	OD1	ASP	B	150	0.093	16.575	24.172	1.00	38.49	
ATOM	4000	OD2	ASP	B	150	0.621	14.450	24.149	1.00	37.98	
ATOM	4001	C	ASP	B	150	-0.673	17.695	21.578	1.00	38.03	
ATOM	4002	O	ASP	B	150	-0.191	18.526	20.803	1.00	35.91	
ATOM	4003	N	VAL	B	151	-1.325	18.036	22.687	1.00	38.58	
ATOM	4004	CA	VAL	B	151	-1.527	19.432	23.055	1.00	38.83	
ATOM	4005	CB	VAL	B	151	-2.403	19.567	24.316	1.00	39.52	
ATOM	4006	CG1	VAL	B	151	-2.705	21.028	24.579	1.00	39.97	
ATOM	4007	CG2	VAL	B	151	-3.678	18.778	24.142	1.00	40.52	
ATOM	4008	C	VAL	B	151	-0.185	20.057	23.331	1.00	38.33	
ATOM	4009	O	VAL	B	151	0.047	21.213	22.982	1.00	38.42	
ATOM	4010	N	ARG	B	152	0.676	19.302	24.012	1.00	37.29	
ATOM	4011	CA	ARG	B	152	2.022	19.761	24.291	1.00	36.95	
ATOM	4012	CB	ARG	B	152	2.718	18.842	25.304	1.00	38.55	
ATOM	4013	CG	ARG	B	152	2.144	18.896	26.717	1.00	40.64	
ATOM	4014	CD	ARG	B	152	0.984	17.935	26.875	1.00	41.39	
ATOM	4015	NE	ARG	B	152	1.454	16.561	27.041	1.00	43.21	
ATOM	4016	CZ	ARG	B	152	0.674	15.492	26.935	1.00	44.44	
ATOM	4017	NH1	ARG	B	152	-0.619	15.645	26.656	1.00	46.42	
ATOM	4018	NH2	ARG	B	152	1.176	14.274	27.116	1.00	43.86	
ATOM	4019	C	ARG	B	152	2.683	19.626	22.921	1.00	36.41	
ATOM	4020	O	ARG	B	152	3.410	18.659	22.678	1.00	34.83	
ATOM	4021	N	TYR	B	153	2.403	20.580	22.031	1.00	34.80	
ATOM	4022	CA	TYR	B	153	2.927	20.555	20.665	1.00	33.74	
ATOM	4023	CB	TYR	B	153	2.686	21.906	19.963	1.00	35.98	
ATOM	4024	CG	TYR	B	153	3.406	23.061	20.611	1.00	38.54	
ATOM	4025	CD1	TYR	B	153	2.975	23.581	21.835	1.00	39.34	
ATOM	4026	CE1	TYR	B	153	3.698	24.581	22.487	1.00	39.67	
ATOM	4027	CD2	TYR	B	153	4.574	23.582	20.049	1.00	39.01	
ATOM	4028	CE2	TYR	B	153	5.310	24.586	20.696	1.00	39.82	
ATOM	4029	CZ	TYR	B	153	4.866	25.075	21.915	1.00	40.12	
ATOM	4030	OH	TYR	B	153	5.607	26.030	22.574	1.00	39.51	
ATOM	4031	C	TYR	B	153	4.403	20.171	20.568	1.00	32.24	
ATOM	4032	O	TYR	B	153	4.833	19.616	19.554	1.00	30.69	
ATOM	4033	N	TYR	B	154	5.175	20.445	21.612	1.00	30.25	
ATOM	4034	CA	TYR	B	154	6.585	20.103	21.597	1.00	30.50	
ATOM	4035	CB	TYR	B	154	7.324	20.751	22.779	1.00	32.66	
ATOM	4036	CG	TYR	B	154	6.785	20.471	24.172	1.00	35.85	
ATOM	4037	CD1	TYR	B	154	7.325	19.450	24.953	1.00	36.54	
ATOM	4038	CE1	TYR	B	154	6.888	19.225	26.267	1.00	37.57	
ATOM	4039	CD2	TYR	B	154	5.779	21.270	24.734	1.00	37.28	
ATOM	4040	CE2	TYR	B	154	5.334	21.053	26.047	1.00	37.15	
ATOM	4041	OH	TYR	B	154	5.895	20.030	26.805	1.00	38.13	
ATOM	4042	C	TYR	B	154	5.477	19.804	28.098	1.00	38.78	
ATOM	4043	O	TYR	B	154	6.813	18.585	21.571	1.00	29.59	
ATOM	4044	N	LEU	B	155	7.817	18.113	21.040	1.00	28.98	
ATOM	4045	CA	LEU	B	155	5.874	17.816	22.109	1.00	27.11	
ATOM	4046	CB	LEU	B	155	6.029	16.359	22.087	1.00	26.11	
ATOM	4047	CG	LEU	B	155	5.055	15.686	23.064	1.00	25.90	
ATOM	4048	CD1	LEU	B	155	5.260	16.046	24.536	1.00	27.10	
ATOM	4049	CD2	LEU	B	155	4.256	15.237	25.360	1.00	29.20	
ATOM	4050	C	LEU	B	155	6.686	15.757	24.980	1.00	28.73	
ATOM	4051	O	LEU	B	155	5.808	15.776	20.682	1.00	25.64	
ATOM	4052	N	ASN	B	156	6.177	14.613	20.431	1.00	25.89	
ATOM	4053	CA	ASN	B	156	5.210	16.560	19.781	1.00	23.01	
ATOM	4054	CB	ASN	B	156	4.962	16.121	18.405	1.00	23.44	
ATOM	4055	CG	ASN	B	156	3.911	16.986	17.737	1.00	25.76	
ATOM	4056	OD1	ASN	B	156	2.570	16.900	18.436	1.00	29.20	
ATOM	4057	ND2	ASN	B	156	1.720	17.790	18.296	1.00	30.71	
ATOM	4058	C	ASN	B	156	2.373	15.830	19.194	1.00	24.28	
ATOM	4059	O	ASN	B	156	6.235	16.141	17.547	1.00	23.66	
ATOM	4060	N	GLY	B	157	6.203	15.696	16.400	1.00	23.58	
ATOM	4061	CA	GLY	B	157	7.332	16.630	18.122	1.00	22.86	
ATOM	4062	C	GLY	B	157	6.596	16.686	17.399	1.00	22.29	
ATOM	4063	O	GLY	B	157	9.630	15.756	18.000	1.00	22.40	
ATOM	4064	N	MET	B	158	9.307	14.894	18.819	1.00	21.77	
ATOM	4065					10.890	15.911	17.604	1.00	19.12	

Figure 1 (continued 41)

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ATOM	4066	CA	MET	B	158	11.963	15.074	18.121	1.00	18.96	B
ATOM	4067	CB	MET	B	158	12.516	14.163	17.003	1.00	16.50	B
ATOM	4068	CG	MET	B	158	13.688	13.297	17.395	1.00	15.32	B
ATOM	4069	SD	MET	B	158	14.254	12.335	16.029	1.00	15.20	B
ATOM	4070	CE	MET	B	158	12.913	10.970	16.029	1.00	15.94	B
ATOM	4071	C	MET	B	158	13.095	15.928	18.658	1.00	19.64	B
ATOM	4072	O	MET	B	158	13.530	16.880	18.006	1.00	18.73	B
ATOM	4073	N	LEU	B	159	13.564	15.621	19.854	1.00	19.03	B
ATOM	4074	CA	LEU	B	159	14.674	16.383	20.397	1.00	19.89	B
ATOM	4075	CB	LEU	B	159	14.747	16.250	21.921	1.00	21.16	B
ATOM	4076	CG	LEU	B	159	15.847	17.145	22.504	1.00	23.17	B
ATOM	4077	CD1	LEU	B	159	15.239	18.525	22.690	1.00	24.44	B
ATOM	4078	CD2	LEU	B	159	16.406	16.575	23.857	1.00	26.60	B
ATOM	4079	C	LEU	B	159	15.999	15.897	19.816	1.00	18.80	B
ATOM	4080	O	LEU	B	159	16.232	14.693	19.707	1.00	19.10	B
ATOM	4081	N	PHE	B	160	16.854	16.844	19.397	1.00	18.54	B
ATOM	4082	CA	PHE	B	160	18.194	16.522	18.906	1.00	18.56	B
ATOM	4083	CB	PHE	B	160	18.414	17.041	17.481	1.00	17.32	B
ATOM	4084	CG	PHE	B	160	17.833	16.158	16.414	1.00	16.68	B
ATOM	4085	CD1	PHE	B	160	16.460	16.129	16.172	1.00	16.33	B
ATOM	4086	CD2	PHE	B	160	18.668	15.338	15.644	1.00	18.29	B
ATOM	4087	CE1	PHE	B	160	15.916	15.291	15.170	1.00	15.09	B
ATOM	4088	CE2	PHE	B	160	18.145	14.498	14.641	1.00	18.37	B
ATOM	4089	CZ	PHE	B	160	16.758	14.474	14.400	1.00	16.02	B
ATOM	4090	C	PHE	B	160	19.169	17.220	19.862	1.00	20.39	B
ATOM	4091	O	PHE	B	160	19.045	18.421	20.088	1.00	22.48	B
ATOM	4092	N	GLU	B	161	20.123	16.472	20.409	1.00	22.11	B
ATOM	4093	CA	GLU	B	161	21.062	17.021	21.371	1.00	23.08	B
ATOM	4094	CB	GLU	B	161	20.595	16.616	22.795	1.00	25.07	B
ATOM	4095	CG	GLU	B	161	21.687	16.649	23.845	1.00	29.45	B
ATOM	4096	CD	GLU	B	161	21.216	16.219	25.237	1.00	32.67	B
ATOM	4097	OE1	GLU	B	161	20.335	15.337	25.350	1.00	33.61	B
ATOM	4098	OE2	GLU	B	161	21.762	16.750	26.232	1.00	35.08	B
ATOM	4099	C	GLU	B	161	22.515	16.620	21.139	1.00	23.37	B
ATOM	4100	O	GLU	B	161	22.817	15.483	20.812	1.00	22.03	B
ATOM	4101	N	THR	B	162	23.422	17.589	21.282	1.00	24.63	B
ATOM	4102	CA	THR	B	162	24.848	17.337	21.145	1.00	26.40	B
ATOM	4103	CB	THR	B	162	25.546	18.444	20.281	1.00	25.08	B
ATOM	4104	OG1	THR	B	162	25.086	19.747	20.676	1.00	24.91	B
ATOM	4105	CG2	THR	B	162	25.223	18.231	18.803	1.00	27.18	B
ATOM	4106	C	THR	B	162	25.438	17.336	22.565	1.00	27.15	B
ATOM	4107	O	THR	B	162	25.127	18.222	23.359	1.00	28.33	B
ATOM	4108	N	GLU	B	163	26.256	16.332	22.881	1.00	29.67	B
ATOM	4109	CA	GLU	B	163	26.883	16.224	24.207	1.00	31.99	B
ATOM	4110	CB	GLU	B	163	25.975	15.463	25.173	1.00	34.55	B
ATOM	4111	CG	GLU	B	163	24.640	16.124	25.426	1.00	37.21	B
ATOM	4112	CD	GLU	B	163	24.739	17.368	26.290	1.00	40.30	B
ATOM	4113	OE1	GLU	B	163	25.272	17.271	27.421	1.00	42.28	B
ATOM	4114	OE2	GLU	B	163	24.272	18.442	25.843	1.00	40.47	B
ATOM	4115	C	GLU	B	163	28.208	15.514	24.119	1.00	31.89	B
ATOM	4116	O	GLU	B	163	28.284	14.360	23.703	1.00	31.49	B
ATOM	4117	N	GLY	B	164	29.263	16.208	24.524	1.00	33.08	B
ATOM	4118	CA	GLY	B	164	30.578	15.612	24.458	1.00	34.03	B
ATOM	4119	C	GLY	B	164	30.958	15.337	23.015	1.00	34.75	B
ATOM	4120	O	GLY	B	164	31.279	16.249	22.251	1.00	35.89	B
ATOM	4121	N	GLU	B	165	30.900	14.070	22.637	1.00	33.48	B
ATOM	4122	CA	GLU	B	165	31.243	13.651	21.296	1.00	33.45	B
ATOM	4123	CB	GLU	B	165	32.465	12.749	21.359	1.00	36.52	B
ATOM	4124	CG	GLU	B	165	32.859	12.136	20.032	1.00	40.64	B
ATOM	4125	CD	GLU	B	165	33.569	10.807	20.209	1.00	41.89	B
ATOM	4126	OE1	GLU	B	165	34.538	10.756	21.003	1.00	45.17	B
ATOM	4127	OE2	GLU	B	165	33.163	9.825	19.552	1.00	42.89	B
ATOM	4128	C	GLU	B	165	30.069	12.886	20.686	1.00	31.49	B
ATOM	4129	O	GLU	B	165	30.216	12.207	19.680	1.00	30.99	B
ATOM	4130	N	GLU	B	166	28.898	12.996	21.301	1.00	31.17	B
ATOM	4131	CA	GLU	B	166	27.734	11.272	20.786	1.00	30.34	B
ATOM	4132	CB	GLU	B	166	27.186	11.327	20.852	1.00	32.23	B
ATOM	4133	CG	GLU	B	166	28.125	10.236	22.339	1.00	35.23	B
ATOM	4134	CD	GLU	B	166	27.417	9.289	23.290	1.00	37.18	B
ATOM	4135	OE1	GLU	B	166	27.041	9.723	24.405	1.00	38.59	B
ATOM	4136	OE2	GLU	B	166	27.218	8.120	22.913	1.00	39.47	B
ATOM	4137	C	GLU	B	166	26.570	13.156	20.329	1.00	27.86	B
ATOM	4138	O	GLU	B	166	26.408	14.273	20.797	1.00	27.41	B
ATOM	4139	N	LEU	B	167	25.776	12.628	19.397	1.00	25.92	B
ATOM	4140	CA	LEU	B	167	24.560	13.291	18.930	1.00	23.86	B
ATOM	4141	CB	LEU	B	167	24.455	13.313	17.402	1.00	23.73	B
ATOM	4142	CG	LEU	B	167	23.631	14.415	16.685	1.00	24.90	B
ATOM	4143	CD1	LEU	B	167	23.059	13.834	15.415	1.00	21.07	B
ATOM	4144	CD2	LEU	B	167	22.555	15.041	17.534	1.00	23.85	B
ATOM	4145	C	LEU	B	167	23.520	12.303	19.481	1.00	21.77	B
ATOM	4146	O	LEU	B	167	23.705	11.083	19.405	1.00	22.32	B
ATOM	4147	N	ARG	B	168	22.439	12.834	20.021	1.00	21.49	B
ATOM	4148	CA	ARG	B	168	21.393	11.996	20.596	1.00	21.70	B
ATOM	4149	CB	ARG	B	168	21.549	12.047	22.117	1.00	24.79	B
ATOM	4150	CG	ARG	B	168	20.309	11.678	22.928	1.00	27.63	B
ATOM	4151	CD	ARG	B	168	20.635	11.575	24.419	1.00	31.15	B
ATOM	4152	NE	ARG	B	168	21.104	12.813	25.018	1.00	33.80	B
ATOM	4153	CZ	ARG	B	168	22.333	13.005	25.502	1.00	33.14	B
ATOM	4154	NH1	ARG	B	168	23.245	12.040	25.466	1.00	33.70	B
ATOM	4155	NH2	ARG	B	168	22.646	14.169	26.022	1.00	34.73	B
ATOM	4156	C	ARG	B	168	20.001	12.475	20.188	1.00	20.94	B
ATOM	4157	O	ARG	B	168	19.782	13.664	19.977	1.00	20.05	B
ATOM	4158	N	THR	B	169	19.059	11.549	20.026	1.00	18.53	B
ATOM	4159	CA	THR	B	169	17.693	11.945	19.748	1.00	17.19	B
ATOM	4160	CB	THR	B	169	17.141	11.377	18.420	1.00	17.29	B
ATOM	4161	OG1	THR	B	169	17.290	9.961	18.415	1.00	17.62	B
ATOM	4162	CG2	THR	B	169	17.936	11.920	17.241	1.00	17.89	B
ATOM	4163	C	THR	B	169	16.846	11.382	20.870	1.00	18.82	B
ATOM	4164	O	THR	B	169	17.200	10.356	21.474	1.00	18.41	B
ATOM	4165	N	VAL	B	170	15.772	12.095	21.151	1.00	18.62	B

Figure 1 (continued 42)

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ATOM	4166	CA	VAL	B	170	14.796	11.705	22.176	1.00	18.28	B
ATOM	4167	CB	VAL	B	170	15.031	12.497	23.489	1.00	17.76	B
ATOM	4168	CG1	VAL	B	170	14.085	11.948	24.589	1.00	18.88	B
ATOM	4169	CG2	VAL	B	170	16.520	12.397	23.913	1.00	18.42	B
ATOM	4170	C	VAL	B	170	13.368	11.981	21.674	1.00	18.46	B
ATOM	4171	O	VAL	B	170	13.087	13.010	21.060	1.00	18.89	B
ATOM	4172	N	ALA	B	171	12.455	11.031	21.908	1.00	15.83	B
ATOM	4173	CA	ALA	B	171	11.069	11.206	21.518	1.00	16.19	B
ATOM	4174	CB	ALA	B	171	10.771	10.503	20.212	1.00	16.47	B
ATOM	4175	C	ALA	B	171	10.234	10.606	22.617	1.00	17.41	B
ATOM	4176	O	ALA	B	171	10.642	9.616	23.213	1.00	18.10	B
ATOM	4177	N	THR	B	172	9.112	11.246	22.902	1.00	16.52	B
ATOM	4178	CA	THR	B	172	8.212	10.730	23.917	1.00	17.52	B
ATOM	4179	CB	THR	B	172	8.776	11.014	25.344	1.00	18.95	B
ATOM	4180	OG1	THR	B	172	7.931	10.400	26.328	1.00	19.33	B
ATOM	4181	CG2	THR	B	172	8.870	12.532	25.619	1.00	18.29	B
ATOM	4182	C	THR	B	172	6.805	11.269	23.709	1.00	18.84	B
ATOM	4183	O	THR	B	172	6.588	12.352	23.145	1.00	20.21	B
ATOM	4184	N	ASP	B	173	5.820	10.481	24.134	1.00	18.12	B
ATOM	4185	CA	ASP	B	173	4.447	10.902	23.972	1.00	19.17	B
ATOM	4186	CB	ASP	B	173	3.709	9.980	22.996	1.00	19.41	B
ATOM	4187	CG	ASP	B	173	3.663	8.531	23.461	1.00	19.37	B
ATOM	4188	OD1	ASP	B	173	4.197	8.212	24.540	1.00	20.26	B
ATOM	4189	OD2	ASP	B	173	3.087	7.712	22.710	1.00	18.53	B
ATOM	4190	C	ASP	B	173	3.766	10.895	25.336	1.00	19.52	B
ATOM	4191	O	ASP	B	173	2.546	11.011	25.408	1.00	22.02	B
ATOM	4192	N	GLY	B	174	4.562	10.770	26.397	1.00	20.37	B
ATOM	4193	CA	GLY	B	174	3.992	10.745	27.737	1.00	22.96	B
ATOM	4194	C	GLY	B	174	3.762	9.337	28.266	1.00	24.51	B
ATOM	4195	O	GLY	B	174	3.667	9.141	29.489	1.00	26.84	B
ATOM	4196	N	HIS	B	175	3.650	8.349	27.375	1.00	23.92	B
ATOM	4197	CA	HIS	B	175	3.440	6.953	27.796	1.00	22.95	B
ATOM	4198	CB	HIS	B	175	2.313	6.309	26.977	1.00	25.89	B
ATOM	4199	CG	HIS	B	175	0.992	6.997	27.119	1.00	28.87	B
ATOM	4200	CD2	HIS	B	175	0.106	7.435	26.193	1.00	30.90	B
ATOM	4201	ND1	HIS	B	175	0.420	7.255	28.345	1.00	30.54	B
ATOM	4202	CE1	HIS	B	175	-0.763	7.817	28.170	1.00	28.94	B
ATOM	4203	NE2	HIS	B	175	-0.977	7.938	26.875	1.00	31.49	B
ATOM	4204	C	HIS	B	175	4.706	6.135	27.641	1.00	23.03	B
ATOM	4205	O	HIS	B	175	4.990	5.212	28.403	1.00	22.08	B
ATOM	4206	N	ARG	B	176	5.481	6.461	26.617	1.00	18.76	B
ATOM	4207	CA	ARG	B	176	6.711	5.768	26.422	1.00	18.30	B
ATOM	4208	CB	ARG	B	176	6.575	4.633	25.398	1.00	19.53	B
ATOM	4209	CG	ARG	B	176	6.329	5.094	23.954	1.00	22.88	B
ATOM	4210	CD	ARG	B	176	4.876	4.888	23.657	1.00	22.11	B
ATOM	4211	NE	ARG	B	176	4.435	5.312	22.314	1.00	22.09	B
ATOM	4212	CZ	ARG	B	176	4.555	4.591	21.202	1.00	20.17	B
ATOM	4213	NH1	ARG	B	176	5.159	3.403	21.213	1.00	17.04	B
ATOM	4214	NH2	ARG	B	176	3.914	4.977	20.120	1.00	20.02	B
ATOM	4215	C	ARG	B	176	7.684	6.807	25.902	1.00	17.30	B
ATOM	4216	O	ARG	B	176	7.255	7.860	25.374	1.00	17.10	B
ATOM	4217	N	LEU	B	177	8.957	6.504	26.080	1.00	17.97	B
ATOM	4218	CA	LEU	B	177	10.049	7.360	25.633	1.00	17.85	B
ATOM	4219	CB	LEU	B	177	10.664	8.095	26.827	1.00	18.29	B
ATOM	4220	CG	LEU	B	177	11.921	8.955	26.611	1.00	16.28	B
ATOM	4221	CD1	LEU	B	177	11.819	10.163	27.559	1.00	19.52	B
ATOM	4222	CD2	LEU	B	177	13.191	8.172	26.839	1.00	19.12	B
ATOM	4223	C	LEU	B	177	11.110	6.517	24.964	1.00	18.45	B
ATOM	4224	O	LEU	B	177	11.291	5.329	25.281	1.00	18.33	B
ATOM	4225	N	ALA	B	178	11.801	7.131	24.006	1.00	15.84	B
ATOM	4226	CA	ALA	B	178	12.899	6.489	23.308	1.00	15.12	B
ATOM	4227	CB	ALA	B	178	12.495	6.133	21.883	1.00	13.82	B
ATOM	4228	C	ALA	B	178	14.041	7.488	23.279	1.00	15.48	B
ATOM	4229	O	ALA	B	178	13.797	8.670	23.063	1.00	17.09	B
ATOM	4230	N	VAL	B	179	15.258	7.014	23.546	1.00	17.40	B
ATOM	4231	CA	VAL	B	179	16.470	7.851	23.508	1.00	18.38	B
ATOM	4232	CB	VAL	B	179	16.881	8.318	24.937	1.00	18.67	B
ATOM	4233	CG1	VAL	B	179	17.294	7.120	25.770	1.00	19.18	B
ATOM	4234	CG2	VAL	B	179	18.060	9.286	24.864	1.00	20.37	B
ATOM	4235	C	VAL	B	179	17.590	7.037	22.849	1.00	19.44	B
ATOM	4236	O	VAL	B	179	17.737	5.829	23.092	1.00	19.37	B
ATOM	4237	N	CYS	B	180	18.370	7.676	21.968	1.00	17.08	B
ATOM	4238	CA	CYS	B	180	19.434	6.979	21.293	1.00	18.58	B
ATOM	4239	CB	CYS	B	180	18.961	6.489	19.918	1.00	17.06	B
ATOM	4240	SG	CYS	B	180	20.198	5.643	18.973	1.00	22.31	B
ATOM	4241	C	CYS	B	180	20.602	7.948	21.135	1.00	19.35	B
ATOM	4242	O	CYS	B	180	20.405	9.093	20.736	1.00	19.68	B
ATOM	4243	N	SER	B	181	21.798	7.464	21.442	1.00	21.74	B
ATOM	4244	CA	SER	B	181	23.015	8.277	21.369	1.00	25.46	B
ATOM	4245	CB	SER	B	181	23.615	8.457	22.774	1.00	28.11	B
ATOM	4246	OG	SER	B	181	22.674	9.033	23.654	1.00	30.74	B
ATOM	4247	C	SER	B	181	24.037	7.590	20.498	1.00	26.06	B
ATOM	4248	O	SER	B	181	24.182	6.370	20.554	1.00	25.12	B
ATOM	4249	N	MET	B	182	24.765	8.374	19.704	1.00	25.90	B
ATOM	4250	CA	MET	B	182	25.779	7.846	18.813	1.00	29.20	B
ATOM	4251	CB	MET	B	182	25.238	7.784	17.382	1.00	31.43	B
ATOM	4252	CG	MET	B	182	24.114	6.789	17.181	1.00	33.69	B
ATOM	4253	SD	MET	B	182	24.722	5.139	17.524	1.00	34.88	B
ATOM	4254	CE	MET	B	182	25.373	4.651	15.929	1.00	34.59	B
ATOM	4255	C	MET	B	182	27.001	8.758	18.834	1.00	30.52	B
ATOM	4256	O	MET	B	182	26.857	9.983	18.819	1.00	30.18	B
ATOM	4257	N	PRO	B	183	28.214	8.177	18.872	1.00	32.39	B
ATOM	4258	CD	PRO	B	183	28.529	6.737	18.860	1.00	34.00	B
ATOM	4259	CA	PRO	B	183	29.449	8.977	18.888	1.00	34.40	B
ATOM	4260	CB	PRO	B	183	30.521	7.940	19.199	1.00	34.66	B
ATOM	4261	CG	PRO	B	183	29.998	6.735	18.481	1.00	35.09	B
ATOM	4262	C	PRO	B	183	29.663	9.624	17.517	1.00	35.33	B
ATOM	4263	O	PRO	B	183	29.355	9.015	16.502	1.00	35.46	B
ATOM	4264	N	ILE	B	184	30.199	10.843	17.506	1.00	36.88	B
ATOM	4265	CA	ILE	B	184	30.445	11.589	16.271	1.00	38.38	B

Figure.1. (continued.43)

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ATOM	4266	CB	ILE	B	184	29.676	12.942	16.305	1.00	37.59	B
ATOM	4267	CG2	ILE	B	184	30.131	13.872	15.192	1.00	39.18	B
ATOM	4268	CG1	ILE	B	184	28.185	12.670	16.154	1.00	39.46	B
ATOM	4269	CD1	ILE	B	184	27.857	11.818	14.939	1.00	38.79	B
ATOM	4270	C	ILE	B	184	31.926	11.864	15.976	1.00	39.26	B
ATOM	4271	O	ILE	B	184	32.266	12.371	14.913	1.00	39.33	B
ATOM	4272	N	GLY	B	185	32.810	11.528	16.906	1.00	40.53	B
ATOM	4273	CA	GLY	B	185	34.225	11.777	16.671	1.00	42.10	B
ATOM	4274	C	GLY	B	185	34.630	13.227	16.897	1.00	43.16	B
ATOM	4275	O	GLY	B	185	35.821	13.542	16.982	1.00	44.33	B
ATOM	4276	N	GLN	B	186	33.646	14.117	16.988	1.00	43.84	B
ATOM	4277	CA	GLN	B	186	33.898	15.541	17.208	1.00	44.08	B
ATOM	4278	CB	GLN	B	186	33.069	16.406	16.254	1.00	43.89	B
ATOM	4279	CG	GLN	B	186	33.456	16.388	14.806	1.00	44.39	B
ATOM	4280	CD	GLN	B	186	32.677	17.426	14.006	1.00	43.95	B
ATOM	4281	O	GLN	B	186	32.773	18.631	14.269	1.00	44.45	B
ATOM	4282	NE2	GLN	B	186	31.893	16.963	13.039	1.00	42.44	B
ATOM	4283	C	GLN	B	186	33.503	15.952	18.614	1.00	44.05	B
ATOM	4284	O	GLN	B	186	32.650	15.325	19.228	1.00	44.15	B
ATOM	4285	N	SER	B	187	34.115	17.019	19.115	1.00	43.83	B
ATOM	4286	CA	SER	B	187	33.779	17.544	20.434	1.00	43.99	B
ATOM	4287	CB	SER	B	187	35.025	18.105	21.138	1.00	44.53	B
ATOM	4288	OG	SER	B	187	36.033	17.117	21.304	1.00	45.53	B
ATOM	4289	C	SER	B	187	32.797	18.675	20.121	1.00	43.54	B
ATOM	4290	O	SER	B	187	33.117	19.573	19.338	1.00	43.42	B
ATOM	4291	N	LEU	B	188	31.603	18.635	20.705	1.00	42.54	B
ATOM	4292	CA	LEU	B	188	30.616	19.669	20.425	1.00	41.93	B
ATOM	4293	CB	LEU	B	188	29.425	19.083	19.652	1.00	42.36	B
ATOM	4294	CG	LEU	B	188	29.558	18.823	18.148	1.00	42.40	B
ATOM	4295	CD1	LEU	B	188	30.321	19.973	17.494	1.00	42.81	B
ATOM	4296	CD2	LEU	B	188	30.269	17.515	17.910	1.00	42.43	B
ATOM	4297	C	LEU	B	188	30.074	20.411	21.623	1.00	41.46	B
ATOM	4298	O	LEU	B	188	30.097	19.910	22.742	1.00	42.28	B
ATOM	4299	N	PRO	B	189	29.580	21.638	21.398	1.00	40.92	B
ATOM	4300	CD	PRO	B	189	29.691	22.410	20.147	1.00	40.91	B
ATOM	4301	CA	PRO	B	189	29.009	22.457	22.466	1.00	39.91	B
ATOM	4302	CB	PRO	B	189	28.784	23.810	21.793	1.00	40.82	B
ATOM	4303	CG	PRO	B	189	29.770	23.819	20.656	1.00	41.55	B
ATOM	4304	C	PRO	B	189	27.683	21.801	22.853	1.00	39.55	B
ATOM	4305	O	PRO	B	189	26.834	21.544	21.995	1.00	37.81	B
ATOM	4306	N	SER	B	190	27.507	21.512	24.134	1.00	38.79	B
ATOM	4307	CA	SER	B	190	26.266	20.889	24.577	1.00	38.03	B
ATOM	4308	CB	SER	B	190	26.237	20.860	26.103	1.00	38.64	B
ATOM	4309	OG	SER	B	190	27.459	20.337	26.593	1.00	41.63	B
ATOM	4310	C	SER	B	190	25.126	21.733	24.005	1.00	36.48	B
ATOM	4311	O	SER	B	190	25.072	22.937	24.221	1.00	37.47	B
ATOM	4312	N	HIS	B	191	24.214	21.102	23.268	1.00	34.74	B
ATOM	4313	CA	HIS	B	191	23.122	21.831	22.620	1.00	32.42	B
ATOM	4314	CB	HIS	B	191	23.568	22.172	21.214	1.00	33.72	B
ATOM	4315	CG	HIS	B	191	23.168	23.535	20.772	1.00	34.73	B
ATOM	4316	CD2	HIS	B	191	22.084	23.968	20.094	1.00	35.24	B
ATOM	4317	ND1	HIS	B	191	23.936	24.649	21.031	1.00	35.16	B
ATOM	4318	CE1	HIS	B	191	23.339	25.714	20.527	1.00	36.06	B
ATOM	4319	NE2	HIS	B	191	22.212	25.328	19.955	1.00	35.42	B
ATOM	4320	C	HIS	B	191	21.803	21.029	22.537	1.00	31.03	B
ATOM	4321	O	HIS	B	191	21.851	19.831	22.375	1.00	31.38	B
ATOM	4322	N	SER	B	192	20.649	21.695	22.605	1.00	29.69	B
ATOM	4323	CA	SER	B	192	19.354	20.993	22.547	1.00	28.86	B
ATOM	4324	CB	SER	B	192	18.819	20.691	23.955	1.00	28.56	B
ATOM	4325	OG	SER	B	192	19.649	19.762	24.617	1.00	32.04	B
ATOM	4326	C	SER	B	192	18.239	21.687	21.801	1.00	28.26	B
ATOM	4327	O	SER	B	192	17.764	22.768	22.223	1.00	29.68	B
ATOM	4328	N	VAL	B	193	17.765	21.042	20.731	1.00	23.60	B
ATOM	4329	CA	VAL	B	193	16.676	21.602	19.942	1.00	22.38	B
ATOM	4330	CB	VAL	B	193	17.198	22.242	18.651	1.00	20.07	B
ATOM	4331	CG1	VAL	B	193	18.139	23.408	18.996	1.00	22.51	B
ATOM	4332	CG2	VAL	B	193	17.914	21.209	17.824	1.00	21.46	B
ATOM	4333	C	VAL	B	193	15.618	20.598	19.542	1.00	21.51	B
ATOM	4334	O	VAL	B	193	15.877	19.389	19.444	1.00	20.75	B
ATOM	4335	N	ILE	B	194	14.431	21.113	19.297	1.00	19.19	B
ATOM	4336	CA	ILE	B	194	13.300	20.279	18.885	1.00	18.69	B
ATOM	4337	CB	ILE	B	194	12.047	20.662	19.661	1.00	20.65	B
ATOM	4338	CG2	ILE	B	194	10.879	19.737	19.263	1.00	20.91	B
ATOM	4339	CG1	ILE	B	194	12.351	20.584	21.156	1.00	22.06	B
ATOM	4340	CD1	ILE	B	194	11.268	21.174	21.991	1.00	25.62	B
ATOM	4341	C	ILE	B	194	13.025	20.452	17.392	1.00	17.66	B
ATOM	4342	O	ILE	B	194	12.699	21.535	16.925	1.00	17.42	B
ATOM	4343	N	VAL	B	195	13.147	19.361	16.641	1.00	17.07	B
ATOM	4344	CA	VAL	B	195	12.878	19.360	15.212	1.00	15.23	B
ATOM	4345	CB	VAL	B	195	13.834	18.401	14.473	1.00	17.30	B
ATOM	4346	CG1	VAL	B	195	13.491	18.338	12.979	1.00	16.64	B
ATOM	4347	CG2	VAL	B	195	15.268	18.857	14.695	1.00	16.68	B
ATOM	4348	C	VAL	B	195	11.412	18.916	15.005	1.00	16.31	B
ATOM	4349	O	VAL	B	195	10.978	17.903	15.567	1.00	16.90	B
ATOM	4350	N	PRO	B	196	10.532	19.670	14.207	1.00	17.47	B
ATOM	4351	CD	PRO	B	196	11.074	20.815	13.395	1.00	18.83	B
ATOM	4352	CA	PRO	B	196	9.215	19.364	13.933	1.00	15.05	B
ATOM	4353	CB	PRO	B	196	8.772	20.478	13.983	1.00	20.57	B
ATOM	4354	CG	PRO	B	196	9.793	21.504	13.114	1.00	22.10	B
ATOM	4355	C	PRO	B	196	9.046	18.009	13.265	1.00	19.72	B
ATOM	4356	O	PRO	B	196	9.944	17.513	12.607	1.00	18.66	B
ATOM	4357	N	ARG	B	197	7.862	17.440	13.430	1.00	20.21	B
ATOM	4358	CA	ARG	B	197	7.519	16.149	12.846	1.00	21.19	B
ATOM	4359	CB	ARG	B	197	6.012	15.904	13.000	1.00	25.71	B
ATOM	4360	CG	ARG	B	197	5.519	14.646	12.322	1.00	30.00	B
ATOM	4361	CD	ARG	B	197	3.984	14.652	12.252	1.00	32.19	B
ATOM	4362	NE	ARG	B	197	3.458	15.525	11.200	1.00	35.51	B
ATOM	4363	CZ	ARG	B	197	3.290	15.155	9.929	1.00	36.04	B
ATOM	4364	NH1	ARG	B	197	3.606	13.925	9.536	1.00	36.85	B
ATOM	4365	NH2	ARG	B	197	2.793	16.012	9.051	1.00	37.72	B

Figure 1 (continued 44)

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ATOM	4366	C	ARG	B	197	7.873	16.032	11.374	1.00	20.20	B
ATOM	4367	O	ARG	B	197	8.529	15.075	10.978	1.00	18.75	B
ATOM	4368	N	LYS	B	198	7.426	16.982	10.553	1.00	19.22	B
ATOM	4369	CA	LYS	B	198	7.713	16.900	9.122	1.00	20.05	B
ATOM	4370	CB	LYS	B	198	6.956	17.965	8.323	1.00	22.68	B
ATOM	4371	CG	LYS	B	198	5.458	17.685	8.160	1.00	27.88	B
ATOM	4372	CD	LYS	B	198	4.815	18.821	7.335	1.00	32.73	B
ATOM	4373	CE	LYS	B	198	3.313	18.648	7.098	1.00	36.66	B
ATOM	4374	NZ	LYS	B	198	2.468	18.767	8.340	1.00	38.58	B
ATOM	4375	O	LYS	B	198	9.190	17.058	8.872	1.00	17.60	B
ATOM	4376	C	LYS	B	198	9.709	16.583	7.873	1.00	19.10	B
ATOM	4377	N	GLY	B	199	9.866	17.731	9.790	1.00	15.43	B
ATOM	4378	CA	GLY	B	199	11.232	17.946	9.628	1.00	16.07	B
ATOM	4379	C	GLY	B	199	12.045	16.641	9.766	1.00	15.66	B
ATOM	4380	O	GLY	B	199	13.015	16.380	9.059	1.00	15.20	B
ATOM	4381	N	VAL	B	200	11.624	15.841	10.737	1.00	14.98	B
ATOM	4382	CA	VAL	B	200	12.245	14.548	10.958	1.00	15.69	B
ATOM	4383	CB	VAL	B	200	11.617	13.864	12.175	1.00	16.41	B
ATOM	4384	CG1	VAL	B	200	12.217	12.449	12.354	1.00	18.05	B
ATOM	4385	CG2	VAL	B	200	11.899	14.718	13.380	1.00	17.11	B
ATOM	4386	C	VAL	B	200	12.056	13.678	9.722	1.00	15.55	B
ATOM	4387	O	VAL	B	200	12.977	12.967	9.284	1.00	17.07	B
ATOM	4388	N	ILE	B	201	10.858	13.703	9.165	1.00	18.07	B
ATOM	4389	CA	ILE	B	201	10.567	12.942	7.950	1.00	18.45	B
ATOM	4390	CB	ILE	B	201	9.084	13.098	7.563	1.00	19.51	B
ATOM	4391	CG2	ILE	B	201	8.814	12.494	6.175	1.00	21.46	B
ATOM	4392	CG1	ILE	B	201	8.238	12.391	8.602	1.00	20.58	B
ATOM	4393	CD1	ILE	B	201	6.738	12.554	8.392	1.00	24.22	B
ATOM	4394	C	ILE	B	201	11.447	13.367	6.789	1.00	18.72	B
ATOM	4395	O	ILE	B	201	11.960	12.519	6.065	1.00	20.22	B
ATOM	4396	N	GLU	B	202	11.643	14.673	6.607	1.00	19.15	B
ATOM	4397	CA	GLU	B	202	12.483	15.152	5.514	1.00	20.05	B
ATOM	4398	CB	GLU	B	202	12.426	16.681	5.362	1.00	21.56	B
ATOM	4399	CG	GLU	B	202	11.174	17.168	4.689	1.00	24.74	B
ATOM	4400	CD	GLU	B	202	10.866	16.349	3.452	1.00	27.41	B
ATOM	4401	OE1	GLU	B	202	9.725	15.850	3.346	1.00	27.85	B
ATOM	4402	OE2	GLU	B	202	11.770	16.185	2.602	1.00	28.02	B
ATOM	4403	C	GLU	B	202	13.923	14.751	5.734	1.00	20.02	B
ATOM	4404	O	GLU	B	202	14.602	14.397	4.773	1.00	21.05	B
ATOM	4405	N	LEU	B	203	14.405	14.838	6.979	1.00	18.48	B
ATOM	4406	CA	LEU	B	203	15.780	14.445	7.272	1.00	19.51	B
ATOM	4407	CB	LEU	B	203	16.102	14.570	8.764	1.00	20.96	B
ATOM	4408	CG	LEU	B	203	16.378	15.983	9.271	1.00	22.79	B
ATOM	4409	CD1	LEU	B	203	16.571	15.960	10.797	1.00	23.58	B
ATOM	4410	CD2	LEU	B	203	17.644	16.526	8.566	1.00	24.88	B
ATOM	4411	C	LEU	B	203	15.987	13.009	6.848	1.00	20.44	B
ATOM	4412	O	LEU	B	203	17.008	12.674	6.231	1.00	18.72	B
ATOM	4413	N	MET	B	204	15.027	12.142	7.171	1.00	18.16	B
ATOM	4414	CA	MET	B	204	15.153	10.734	6.784	1.00	21.15	B
ATOM	4415	CB	MET	B	204	14.008	9.914	7.399	1.00	23.53	B
ATOM	4416	CG	MET	B	204	13.959	8.461	6.938	1.00	29.56	B
ATOM	4417	SD	MET	B	204	15.384	7.475	7.480	1.00	38.65	B
ATOM	4418	CE	MET	B	204	15.782	8.308	8.992	1.00	30.14	B
ATOM	4419	C	MET	B	204	15.147	10.530	5.265	1.00	22.14	B
ATOM	4420	O	MET	B	204	15.920	9.728	4.732	1.00	22.11	B
ATOM	4421	N	ARG	B	205	14.278	11.264	4.579	1.00	22.90	B
ATOM	4422	CA	ARG	B	205	14.147	11.174	3.132	1.00	25.90	B
ATOM	4423	CB	ARG	B	205	13.008	12.052	2.631	1.00	28.24	B
ATOM	4424	CG	ARG	B	205	11.659	11.451	2.747	1.00	31.40	B
ATOM	4425	CD	ARG	B	205	10.612	12.462	2.312	1.00	33.52	B
ATOM	4426	NE	ARG	B	205	9.282	11.913	2.527	1.00	34.98	B
ATOM	4427	CZ	ARG	B	205	8.155	12.614	2.484	1.00	36.39	B
ATOM	4428	NH1	ARG	B	205	8.186	13.912	2.228	1.00	36.54	B
ATOM	4429	NH2	ARG	B	205	6.997	12.008	2.717	1.00	36.70	B
ATOM	4430	C	ARG	B	205	15.360	11.583	2.355	1.00	26.12	B
ATOM	4431	O	ARG	B	205	15.548	11.131	1.226	1.00	25.57	B
ATOM	4432	N	MET	B	206	16.182	12.453	2.923	1.00	25.37	B
ATOM	4433	CA	MET	B	206	17.332	12.907	2.167	1.00	26.52	B
ATOM	4434	CB	MET	B	206	17.690	14.334	2.563	1.00	27.58	B
ATOM	4435	CG	MET	B	206	18.358	14.497	3.881	1.00	25.49	B
ATOM	4436	SD	MET	B	206	18.341	16.237	4.294	1.00	27.01	B
ATOM	4437	CE	MET	B	206	18.905	16.967	2.700	1.00	25.57	B
ATOM	4438	C	MET	B	206	18.541	12.008	2.269	1.00	27.45	B
ATOM	4439	O	MET	B	206	19.584	12.282	1.669	1.00	26.91	B
ATOM	4440	N	LEU	B	207	18.407	10.934	3.036	1.00	28.07	B
ATOM	4441	CA	LEU	B	207	19.512	10.010	3.172	1.00	30.58	B
ATOM	4442	CB	LEU	B	207	19.407	9.290	4.512	1.00	29.11	B
ATOM	4443	CG	LEU	B	207	19.312	10.219	5.724	1.00	26.96	B
ATOM	4444	CD1	LEU	B	207	19.271	9.343	6.995	1.00	27.09	B
ATOM	4445	CD2	LEU	B	207	20.482	11.190	5.763	1.00	24.96	B
ATOM	4446	C	LEU	B	207	19.442	9.029	2.000	1.00	33.44	B
ATOM	4447	O	LEU	B	207	18.468	8.306	1.835	1.00	34.23	B
ATOM	4448	N	ASP	B	208	20.476	9.020	1.170	1.00	37.29	B
ATOM	4449	CA	ASP	B	208	20.490	8.136	0.016	1.00	40.97	B
ATOM	4450	CB	ASP	B	208	21.349	8.726	-1.099	1.00	42.41	B
ATOM	4451	CG	ASP	B	208	22.832	8.627	-0.799	1.00	43.64	B
ATOM	4452	OD1	ASP	B	208	23.355	9.451	-0.024	1.00	45.03	B
ATOM	4453	OD2	ASP	B	208	23.483	7.705	-1.330	1.00	46.54	B
ATOM	4454	N	ASP	B	208	21.079	6.806	0.437	1.00	42.45	B
ATOM	4455	O	ASP	B	208	20.948	5.805	-0.266	1.00	44.07	B
ATOM	4456	C	GLY	B	209	21.728	6.795	1.593	1.00	43.63	B
ATOM	4457	CA	GLY	B	209	22.347	5.573	2.055	1.00	45.09	B
ATOM	4458	CB	GLY	B	209	23.590	5.341	1.220	1.00	45.45	B
ATOM	4459	O	GLY	B	209	23.921	4.207	0.865	1.00	46.37	B
ATOM	4460	N	GLY	B	210	24.273	6.434	0.892	1.00	45.49	B
ATOM	4461	CA	GLY	B	210	25.489	6.350	0.111	1.00	44.86	B
ATOM	4462	C	GLY	B	210	26.648	6.835	0.952	1.00	44.61	B
ATOM	4463	O	GLY	B	210	26.506	7.031	2.158	1.00	44.29	B
ATOM	4464	N	ASP	B	211	27.793	7.036	0.311	1.00	44.84	B
ATOM	4465	CA	ASP	B	211	28.998	7.499	0.985	1.00	44.68	B

Figure 1 (continued 45)

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ATOM	4466	CB	ASP	B	211	30.220	7.108	0.154	1.00	46.96	B
ATOM	4467	CG	ASP	B	211	30.015	7.377	-1.327	1.00	49.59	B
ATOM	4468	OD1	ASP	B	211	29.929	8.365	-1.718	1.00	51.33	B
ATOM	4469	OD2	ASP	B	211	29.924	6.398	-2.100	1.00	51.23	B
ATOM	4470	C	ASP	B	211	29.023	9.008	1.253	1.00	43.00	B
ATOM	4471	O	ASP	B	211	29.901	9.493	1.970	1.00	42.86	B
ATOM	4472	N	ASN	B	212	28.082	9.758	0.679	1.00	40.95	B
ATOM	4473	CA	ASN	B	212	28.054	11.201	0.917	1.00	38.13	B
ATOM	4474	CB	ASN	B	212	26.875	11.872	0.200	1.00	40.65	B
ATOM	4475	CG	ASN	B	212	26.909	11.679	-1.298	1.00	42.99	B
ATOM	4476	OD1	ASN	B	212	26.795	10.553	-1.799	1.00	46.74	B
ATOM	4477	ND2	ASN	B	212	27.064	12.774	-2.026	1.00	43.95	B
ATOM	4478	C	ASN	B	212	27.891	11.442	2.417	1.00	35.10	B
ATOM	4479	O	ASN	B	212	27.031	10.845	3.062	1.00	34.26	B
ATOM	4480	N	PRO	B	213	28.722	12.313	2.992	1.00	32.02	B
ATOM	4481	CD	PRO	B	213	29.862	13.029	2.379	1.00	33.01	B
ATOM	4482	CA	PRO	B	213	28.622	12.604	4.422	1.00	29.13	B
ATOM	4483	CB	PRO	B	213	29.993	13.183	4.742	1.00	31.02	B
ATOM	4484	CG	PRO	B	213	30.301	13.958	3.492	1.00	31.64	B
ATOM	4485	O	PRO	B	213	27.493	13.627	4.641	1.00	26.76	B
ATOM	4486	C	PRO	B	213	27.099	14.330	3.711	1.00	25.59	B
ATOM	4487	N	LEU	B	214	26.964	13.676	5.856	1.00	23.19	B
ATOM	4488	CA	LEU	B	214	25.892	14.608	6.189	1.00	22.69	B
ATOM	4489	CB	LEU	B	214	24.805	13.875	7.006	1.00	25.15	B
ATOM	4490	CG	LEU	B	214	23.706	14.726	7.624	1.00	27.21	B
ATOM	4491	CD1	LEU	B	214	22.868	15.298	6.520	1.00	28.20	B
ATOM	4492	CD2	LEU	B	214	22.840	13.877	8.557	1.00	27.67	B
ATOM	4493	C	LEU	B	214	26.465	15.766	6.993	1.00	21.63	B
ATOM	4494	O	LEU	B	214	27.109	15.551	8.008	1.00	22.98	B
ATOM	4495	N	ARG	B	215	26.255	17.004	6.540	1.00	20.26	B
ATOM	4496	CA	ARG	B	215	26.763	18.148	7.275	1.00	20.31	B
ATOM	4497	CB	ARG	B	215	27.529	19.121	6.367	1.00	24.44	B
ATOM	4498	CG	ARG	B	215	28.163	20.269	7.151	1.00	28.96	B
ATOM	4499	CD	ARG	B	215	29.021	21.199	6.288	1.00	34.52	B
ATOM	4500	NE	ARG	B	215	28.826	22.593	6.691	1.00	38.13	B
ATOM	4501	CZ	ARG	B	215	28.386	23.555	5.879	1.00	39.89	B
ATOM	4502	NH1	ARG	B	215	28.100	23.297	4.605	1.00	41.19	B
ATOM	4503	NH2	ARG	B	215	28.197	24.775	6.352	1.00	42.36	B
ATOM	4504	C	ARG	B	215	25.607	18.863	7.923	1.00	19.25	B
ATOM	4505	O	ARG	B	215	24.672	19.274	7.253	1.00	19.32	B
ATOM	4506	N	VAL	B	216	25.702	19.027	9.231	1.00	16.59	B
ATOM	4507	CA	VAL	B	216	24.645	19.655	10.002	1.00	16.36	B
ATOM	4508	CB	VAL	B	216	24.224	18.737	11.177	1.00	15.73	B
ATOM	4509	CG1	VAL	B	216	23.045	19.383	11.949	1.00	16.54	B
ATOM	4510	CG2	VAL	B	216	23.924	17.379	10.674	1.00	16.55	B
ATOM	4511	C	VAL	B	216	25.029	20.994	10.583	1.00	18.40	B
ATOM	4512	O	VAL	B	216	26.137	21.168	11.094	1.00	18.97	B
ATOM	4513	N	GLN	B	217	24.104	21.951	10.521	1.00	16.54	B
ATOM	4514	CA	GLN	B	217	24.331	23.265	11.096	1.00	18.52	B
ATOM	4515	CB	GLN	B	217	24.482	24.346	10.021	1.00	19.71	B
ATOM	4516	CG	GLN	B	217	25.754	24.294	9.206	1.00	21.74	B
ATOM	4517	CD	GLN	B	217	25.778	25.415	8.168	1.00	24.98	B
ATOM	4518	OE1	GLN	B	217	26.529	26.403	8.299	1.00	28.72	B
ATOM	4519	NE2	GLN	B	217	24.932	25.283	7.141	1.00	23.49	B
ATOM	4520	C	GLN	B	217	23.088	23.566	11.929	1.00	18.28	B
ATOM	4521	O	GLN	B	217	21.970	23.360	11.466	1.00	17.82	B
ATOM	4522	N	ILE	B	218	23.293	23.999	13.170	1.00	17.89	B
ATOM	4523	CA	ILE	B	218	22.184	24.327	14.049	1.00	18.52	B
ATOM	4524	CB	ILE	B	218	22.125	23.382	15.290	1.00	19.36	B
ATOM	4525	CG2	ILE	B	218	20.877	23.687	16.133	1.00	21.63	B
ATOM	4526	CG1	ILE	B	218	22.098	21.932	14.849	1.00	19.21	B
ATOM	4527	CD1	ILE	B	218	22.008	20.959	16.021	1.00	19.55	B
ATOM	4528	C	ILE	B	218	22.333	25.745	14.567	1.00	19.93	B
ATOM	4529	N	ILE	B	218	23.418	26.145	15.038	1.00	18.55	B
ATOM	4530	O	GLY	B	219	21.231	26.488	14.485	1.00	18.45	B
ATOM	4531	CA	GLY	B	219	21.173	27.845	14.966	1.00	20.72	B
ATOM	4532	CB	GLY	B	219	20.113	27.895	16.139	1.00	21.48	B
ATOM	4533	O	GLY	B	219	19.724	26.859	16.621	1.00	20.11	B
ATOM	4534	N	SER	B	220	19.917	29.104	16.597	1.00	23.01	B
ATOM	4535	CA	SER	B	220	19.014	29.266	17.724	1.00	23.61	B
ATOM	4536	CB	SER	B	220	19.009	30.718	18.199	1.00	26.05	B
ATOM	4537	CG	SER	B	220	18.517	31.556	17.166	1.00	29.78	B
ATOM	4538	C	SER	B	220	17.593	28.866	17.345	1.00	23.25	B
ATOM	4539	O	SER	B	220	16.825	28.449	18.203	1.00	21.92	B
ATOM	4540	N	ASN	B	221	17.240	28.989	16.068	1.00	21.87	B
ATOM	4541	CA	ASN	B	221	15.879	28.662	15.667	1.00	21.62	B
ATOM	4542	CB	ASN	B	221	15.065	29.948	15.549	1.00	25.88	B
ATOM	4543	CG	ASN	B	221	15.037	30.730	16.850	1.00	30.93	B
ATOM	4544	OD1	ASN	B	221	15.890	31.585	17.095	1.00	35.31	B
ATOM	4545	ND2	ASN	B	221	14.067	30.423	17.700	1.00	32.95	B
ATOM	4546	C	ASN	B	221	15.750	27.880	14.378	1.00	18.27	B
ATOM	4547	O	ASN	B	221	14.657	27.787	13.830	1.00	18.70	B
ATOM	4548	N	ASN	B	222	16.844	27.284	13.919	1.00	18.16	B
ATOM	4549	CA	ASN	B	222	16.822	26.555	12.653	1.00	16.52	B
ATOM	4550	CB	ASN	B	222	17.258	27.445	11.472	1.00	19.66	B
ATOM	4551	CG	ASN	B	222	16.359	28.636	11.258	1.00	21.30	B
ATOM	4552	OD1	ASN	B	222	16.377	29.589	12.038	1.00	23.15	B
ATOM	4553	ND2	ASN	B	222	15.570	28.607	10.172	1.00	22.47	B
ATOM	4554	C	ASN	B	222	17.820	25.447	12.674	1.00	15.05	B
ATOM	4555	O	ASN	B	222	18.762	25.461	13.464	1.00	15.87	B
ATOM	4556	N	ILE	B	223	17.571	24.457	11.836	1.00	14.78	B
ATOM	4557	CA	ILE	B	223	18.531	23.373	11.657	1.00	13.60	B
ATOM	4558	CB	ILE	B	223	18.077	22.036	12.294	1.00	13.56	B
ATOM	4559	CG2	ILE	B	223	16.722	21.592	11.714	1.00	14.77	B
ATOM	4560	CG1	ILE	B	223	19.172	20.962	12.069	1.00	15.05	B
ATOM	4561	CD1	ILE	B	223	18.996	19.763	13.023	1.00	17.92	B
ATOM	4562	C	ILE	B	223	18.638	23.212	10.158	1.00	15.44	B
ATOM	4563	O	ILE	B	223	17.641	23.372	9.433	1.00	15.61	B
ATOM	4564	N	ARG	B	224	19.860	22.950	9.685	1.00	15.47	B
ATOM	4565	CA	ARG	B	224	20.103	22.744	8.267	1.00	14.89	B

Figure 1 (continued 46)

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ATOM	4566	CB	ARG	B	224	20.845	23.962	7.665	1.00	15.96	B
ATOM	4567	CG	ARG	B	224	21.308	23.736	6.237	1.00	17.14	B
ATOM	4568	CD	ARG	B	224	21.764	25.058	5.624	1.00	19.60	B
ATOM	4569	NE	ARG	B	224	20.628	25.953	5.409	1.00	21.62	B
ATOM	4570	CZ	ARG	B	224	20.704	27.193	4.920	1.00	25.09	B
ATOM	4571	NH1	ARG	B	224	21.882	27.726	4.589	1.00	26.00	B
ATOM	4572	NH2	ARG	B	224	19.594	27.897	4.739	1.00	25.58	B
ATOM	4573	C	ARG	B	224	20.936	21.495	8.092	1.00	14.76	B
ATOM	4574	O	ARG	B	224	21.838	21.212	8.896	1.00	16.22	B
ATOM	4575	N	ALA	B	225	20.611	20.724	7.070	1.00	13.02	B
ATOM	4576	CA	ALA	B	225	21.362	19.518	6.742	1.00	15.06	B
ATOM	4577	CB	ALA	B	225	20.566	18.273	7.054	1.00	14.63	B
ATOM	4578	C	ALA	B	225	21.717	19.524	5.269	1.00	16.06	B
ATOM	4579	O	ALA	B	225	20.865	19.761	4.399	1.00	15.83	B
ATOM	4580	N	HIS	B	226	22.982	19.229	4.992	1.00	16.22	B
ATOM	4581	CA	HIS	B	226	23.470	19.183	3.609	1.00	16.96	B
ATOM	4582	CB	HIS	B	226	24.703	20.072	3.438	1.00	20.34	B
ATOM	4583	CG	HIS	B	226	24.570	21.455	3.984	1.00	22.82	B
ATOM	4584	CD2	HIS	B	226	24.412	21.911	5.251	1.00	25.71	B
ATOM	4585	ND1	HIS	B	226	24.731	22.573	3.193	1.00	26.34	B
ATOM	4586	CE1	HIS	B	226	24.685	23.657	3.947	1.00	25.51	B
ATOM	4587	NE2	HIS	B	226	24.494	23.283	5.199	1.00	26.67	B
ATOM	4588	C	HIS	B	226	23.928	17.756	3.288	1.00	17.69	B
ATOM	4589	O	HIS	B	226	24.739	17.195	4.031	1.00	18.01	B
ATOM	4590	N	VAL	B	227	23.420	17.177	2.203	1.00	16.43	B
ATOM	4591	CA	VAL	B	227	23.829	15.846	1.744	1.00	18.02	B
ATOM	4592	CB	VAL	B	227	22.774	14.737	2.022	1.00	21.51	B
ATOM	4593	CG1	VAL	B	227	23.362	13.373	1.650	1.00	22.64	B
ATOM	4594	CG2	VAL	B	227	22.335	14.777	3.508	1.00	24.44	B
ATOM	4595	C	VAL	B	227	23.944	15.953	0.236	1.00	18.76	B
ATOM	4596	O	VAL	B	227	22.966	16.286	-0.433	1.00	17.98	B
ATOM	4597	N	GLY	B	228	25.117	15.673	-0.323	1.00	18.52	B
ATOM	4598	CA	GLY	B	228	25.233	15.764	-1.768	1.00	18.19	B
ATOM	4599	C	GLY	B	228	24.830	17.146	-2.244	1.00	17.69	B
ATOM	4600	O	GLY	B	228	25.267	18.161	-1.704	1.00	17.83	B
ATOM	4601	N	ASP	B	229	23.945	17.180	-3.231	1.00	17.92	B
ATOM	4602	CA	ASP	B	229	23.548	18.464	-3.754	1.00	17.89	B
ATOM	4603	CB	ASP	B	229	23.598	18.416	-5.278	1.00	20.23	B
ATOM	4604	CG	ASP	B	229	25.018	18.203	-5.796	1.00	24.39	B
ATOM	4605	OD1	ASP	B	229	25.930	18.937	-5.365	1.00	27.15	B
ATOM	4606	OD2	ASP	B	229	25.218	17.308	-6.638	1.00	28.68	B
ATOM	4607	C	ASP	B	229	22.202	18.935	-3.259	1.00	17.01	B
ATOM	4608	O	ASP	B	229	21.532	19.734	-3.937	1.00	16.40	B
ATOM	4609	N	PHE	B	230	21.841	18.485	-2.052	1.00	15.16	B
ATOM	4610	CA	PHE	B	230	20.563	18.856	-1.404	1.00	16.26	B
ATOM	4611	CB	PHE	B	230	19.715	17.622	-1.099	1.00	15.55	B
ATOM	4612	CG	PHE	B	230	19.207	16.943	-2.294	1.00	21.50	B
ATOM	4613	CD1	PHE	B	230	18.078	17.408	-2.938	1.00	21.49	B
ATOM	4614	CD2	PHE	B	230	19.857	15.839	-2.794	1.00	21.72	B
ATOM	4615	CE1	PHE	B	230	17.605	16.756	-4.093	1.00	22.44	B
ATOM	4616	CE2	PHE	B	230	19.390	15.186	-3.940	1.00	24.25	B
ATOM	4617	CZ	PHE	B	230	18.278	15.638	-4.582	1.00	19.43	B
ATOM	4618	C	PHE	B	230	20.816	19.547	-0.102	1.00	15.83	B
ATOM	4619	O	PHE	B	230	21.745	19.203	0.624	1.00	16.68	B
ATOM	4620	N	ILE	B	231	20.006	20.559	0.185	1.00	15.42	B
ATOM	4621	CA	ILE	B	231	20.125	21.288	1.419	1.00	15.06	B
ATOM	4622	CB	ILE	B	231	20.658	22.707	1.197	1.00	17.17	B
ATOM	4623	CG2	ILE	B	231	20.842	23.403	2.547	1.00	17.21	B
ATOM	4624	CG1	ILE	B	231	21.945	22.641	0.378	1.00	19.39	B
ATOM	4625	CD1	ILE	B	231	23.020	21.819	0.992	1.00	27.13	B
ATOM	4626	C	ILE	B	231	18.737	21.413	2.019	1.00	16.11	B
ATOM	4627	O	ILE	B	231	17.839	22.016	1.414	1.00	16.41	B
ATOM	4628	N	PHE	B	232	18.564	20.830	3.196	1.00	13.24	B
ATOM	4629	CA	PHE	B	232	17.287	20.911	3.881	1.00	13.91	B
ATOM	4630	CB	PHE	B	232	16.906	19.529	4.423	1.00	13.73	B
ATOM	4631	CG	PHE	B	232	15.697	19.553	5.287	1.00	15.40	B
ATOM	4632	CD1	PHE	B	232	14.469	19.868	4.725	1.00	15.78	B
ATOM	4633	CD2	PHE	B	232	15.785	19.281	6.642	1.00	16.56	B
ATOM	4634	CE1	PHE	B	232	13.307	19.911	5.522	1.00	18.04	B
ATOM	4635	CE2	PHE	B	232	14.635	19.317	7.459	1.00	18.76	B
ATOM	4636	CZ	PHE	B	232	13.398	19.629	6.892	1.00	16.42	B
ATOM	4637	C	PHE	B	232	17.399	21.890	5.056	1.00	13.92	B
ATOM	4638	O	PHE	B	232	18.365	21.849	5.819	1.00	13.17	B
ATOM	4639	N	THR	B	233	16.421	22.790	5.219	1.00	12.41	B
ATOM	4640	CA	THR	B	233	16.459	23.718	6.340	1.00	12.88	B
ATOM	4641	CB	THR	B	233	16.768	25.163	5.894	1.00	14.92	B
ATOM	4642	CG1	THR	B	233	17.997	25.186	5.150	1.00	16.97	B
ATOM	4643	CG2	THR	B	233	16.957	26.045	7.122	1.00	15.17	B
ATOM	4644	C	THR	B	233	15.097	23.743	7.014	1.00	15.12	B
ATOM	4645	O	THR	B	233	14.086	23.800	6.338	1.00	15.11	B
ATOM	4646	N	SER	B	234	15.058	23.682	8.343	1.00	14.12	B
ATOM	4647	CA	SER	B	234	13.752	23.754	9.028	1.00	14.24	B
ATOM	4648	CB	SER	B	234	13.345	22.386	9.589	1.00	14.75	B
ATOM	4649	CG	SER	B	234	12.055	22.447	10.269	1.00	15.57	B
ATOM	4650	C	SER	B	234	13.799	24.697	10.218	1.00	15.61	B
ATOM	4651	O	SER	B	234	14.848	24.855	10.875	1.00	15.62	B
ATOM	4652	N	LYS	B	235	12.668	25.318	10.511	1.00	15.65	B
ATOM	4653	CA	LYS	B	235	12.614	26.103	11.724	1.00	16.12	B
ATOM	4654	CB	LYS	B	235	11.399	27.058	11.698	1.00	20.85	B
ATOM	4655	CG	LYS	B	235	11.492	28.065	10.552	1.00	22.12	B
ATOM	4656	CD	LYS	B	235	10.989	29.480	10.902	1.00	29.55	B
ATOM	4657	CE	LYS	B	235	9.573	29.464	11.445	1.00	31.45	B
ATOM	4658	NZ	LYS	B	235	8.906	30.815	11.360	1.00	30.18	B
ATOM	4659	C	LYS	B	235	12.482	25.057	12.855	1.00	14.05	B
ATOM	4660	O	LYS	B	235	11.991	23.940	12.643	1.00	16.41	B
ATOM	4661	N	LEU	B	236	12.945	25.430	14.044	1.00	15.37	B
ATOM	4662	CA	LEU	B	236	12.882	24.571	15.220	1.00	15.37	B
ATOM	4663	CB	LEU	B	236	14.087	24.837	16.110	1.00	15.88	B
ATOM	4664	CG	LEU	B	236	15.463	24.474	15.507	1.00	15.11	B
ATOM	4665	CD1	LEU	B	236	16.608	24.944	16.431	1.00	16.66	B

Figure 1 (continued 47)

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ATOM	4666	CD2	LEU	B	236	15.474	22.974	15.228	1.00	16.38	B
ATOM	4667	C	LEU	B	236	11.594	24.879	15.982	1.00	18.39	B
ATOM	4668	O	LEU	B	236	10.986	25.947	15.802	1.00	19.38	B
ATOM	4669	N	VAL	B	237	11.185	23.941	16.831	1.00	21.05	B
ATOM	4670	CA	VAL	B	237	9.983	24.091	17.638	1.00	23.90	B
ATOM	4671	CB	VAL	B	237	9.278	22.707	17.848	1.00	24.44	B
ATOM	4672	CG1	VAL	B	237	8.085	22.831	18.837	1.00	25.05	B
ATOM	4673	CG2	VAL	B	237	8.774	22.189	16.503	1.00	26.22	B
ATOM	4674	C	VAL	B	237	10.380	24.655	19.000	1.00	26.41	B
ATOM	4675	O	VAL	B	237	11.366	24.235	19.589	1.00	25.35	B
ATOM	4676	N	ASP	B	238	9.639	25.636	19.496	1.00	32.01	B
ATOM	4677	CA	ASP	B	238	9.975	26.158	20.816	1.00	37.53	B
ATOM	4678	CB	ASP	B	238	9.528	27.603	20.977	1.00	40.37	B
ATOM	4679	CG	ASP	B	238	10.234	28.530	20.022	1.00	42.20	B
ATOM	4680	OD1	ASP	B	238	11.453	28.325	19.791	1.00	43.09	B
ATOM	4681	OD2	ASP	B	238	9.571	29.466	19.514	1.00	45.01	B
ATOM	4682	C	ASP	B	238	9.284	25.302	21.852	1.00	39.40	B
ATOM	4683	O	ASP	B	238	8.449	24.457	21.519	1.00	41.81	B
ATOM	4684	N	GLY	B	239	9.638	25.498	23.111	1.00	41.31	B
ATOM	4685	CA	GLY	B	239	9.004	24.722	24.157	1.00	42.54	B
ATOM	4686	C	GLY	B	239	10.019	24.022	25.019	1.00	43.17	B
ATOM	4687	O	GLY	B	239	11.188	23.944	24.665	1.00	42.73	B
ATOM	4688	N	ARG	B	240	9.572	23.506	26.156	1.00	44.77	B
ATOM	4689	CA	ARG	B	240	10.473	22.812	27.062	1.00	45.41	B
ATOM	4690	CB	ARG	B	240	10.215	23.260	28.497	1.00	47.67	B
ATOM	4691	CG	ARG	B	240	8.807	22.985	28.997	1.00	50.38	B
ATOM	4692	CD	ARG	B	240	8.662	23.521	30.408	1.00	52.39	B
ATOM	4693	NE	ARG	B	240	8.988	24.942	30.464	1.00	53.18	B
ATOM	4694	CZ	ARG	B	240	9.345	25.580	31.572	1.00	54.35	B
ATOM	4695	NH1	ARG	B	240	9.422	24.925	32.727	1.00	53.83	B
ATOM	4696	NH2	ARG	B	240	9.638	26.871	31.517	1.00	55.03	B
ATOM	4697	C	ARG	B	240	10.277	21.306	26.942	1.00	44.25	B
ATOM	4698	O	ARG	B	240	9.199	20.790	27.237	1.00	45.09	B
ATOM	4699	N	PHE	B	241	11.331	20.615	26.520	1.00	42.31	B
ATOM	4700	CA	PHE	B	241	11.290	19.167	26.326	1.00	40.40	B
ATOM	4701	CB	PHE	B	241	12.024	18.818	25.019	1.00	37.04	B
ATOM	4702	CG	PHE	B	241	11.584	17.518	24.380	1.00	33.05	B
ATOM	4703	CD1	PHE	B	241	12.109	16.303	24.798	1.00	32.26	B
ATOM	4704	CD2	PHE	B	241	10.666	17.529	23.338	1.00	30.96	B
ATOM	4705	CE1	PHE	B	241	11.727	15.108	24.179	1.00	29.39	B
ATOM	4706	CE2	PHE	B	241	10.276	16.347	22.714	1.00	29.62	B
ATOM	4707	CZ	PHE	B	241	10.814	15.134	23.141	1.00	28.51	B
ATOM	4708	C	PHE	B	241	11.892	18.398	27.511	1.00	39.78	B
ATOM	4709	O	PHE	B	241	12.919	18.785	28.077	1.00	40.91	B
ATOM	4710	N	PRO	B	242	11.254	17.279	27.890	1.00	38.82	B
ATOM	4711	CD	PRO	B	242	9.987	16.826	27.286	1.00	37.70	B
ATOM	4712	CA	PRO	B	242	11.660	16.404	28.997	1.00	37.16	B
ATOM	4713	CB	PRO	B	242	10.688	15.230	28.874	1.00	37.98	B
ATOM	4714	CG	PRO	B	242	9.448	15.869	28.336	1.00	37.43	B
ATOM	4715	C	PRO	B	242	13.124	15.947	28.987	1.00	36.91	B
ATOM	4716	O	PRO	B	242	13.728	15.748	27.925	1.00	35.36	B
ATOM	4717	N	ASP	B	243	13.675	15.763	30.184	1.00	35.76	B
ATOM	4718	CA	ASP	B	243	15.053	15.323	30.369	1.00	36.57	B
ATOM	4719	CB	ASP	B	243	15.625	15.957	31.639	1.00	35.26	B
ATOM	4720	CG	ASP	B	243	17.064	15.549	31.907	1.00	36.71	B
ATOM	4721	OD1	ASP	B	243	17.556	14.587	31.281	1.00	36.01	B
ATOM	4722	OD2	ASP	B	243	17.709	16.188	32.767	1.00	36.91	B
ATOM	4723	C	ASP	B	243	15.114	13.796	30.495	1.00	36.45	B
ATOM	4724	O	ASP	B	243	14.919	13.251	31.576	1.00	36.71	B
ATOM	4725	N	TYR	B	244	15.419	13.103	29.407	1.00	36.69	B
ATOM	4726	CA	TYR	B	244	15.477	11.638	29.446	1.00	36.02	B
ATOM	4727	CB	TYR	B	244	16.148	11.089	28.186	1.00	34.53	B
ATOM	4728	CG	TYR	B	244	17.657	10.998	28.255	1.00	34.00	B
ATOM	4729	CD1	TYR	B	244	18.462	12.105	27.968	1.00	32.87	B
ATOM	4730	CD2	TYR	B	244	19.858	12.000	27.984	1.00	34.13	B
ATOM	4731	CE1	TYR	B	244	18.281	9.791	28.566	1.00	33.14	B
ATOM	4732	CE2	TYR	B	244	19.665	9.673	28.581	1.00	34.72	B
ATOM	4733	CZ	TYR	B	244	20.449	10.783	28.283	1.00	34.56	B
ATOM	4734	OH	TYR	B	244	21.811	10.633	28.235	1.00	36.14	B
ATOM	4735	C	TYR	B	244	16.199	11.060	30.673	1.00	37.56	B
ATOM	4736	O	TYR	B	244	15.795	10.029	31.215	1.00	36.17	B
ATOM	4737	N	ARG	B	245	17.269	11.728	31.092	1.00	38.21	B
ATOM	4738	CA	ARG	B	245	18.074	11.296	32.531	1.00	40.14	B
ATOM	4739	CB	ARG	B	245	19.166	12.333	32.519	1.00	40.81	B
ATOM	4740	CG	ARG	B	245	20.029	12.665	31.319	1.00	43.08	B
ATOM	4741	CD	ARG	B	245	21.075	13.731	31.631	1.00	43.61	B
ATOM	4742	NE	ARG	B	245	21.787	14.137	30.420	1.00	45.10	B
ATOM	4743	CZ	ARG	B	245	21.231	14.807	29.413	1.00	45.50	B
ATOM	4744	NH1	ARG	B	245	19.952	15.157	29.464	1.00	44.89	B
ATOM	4745	NH2	ARG	B	245	21.956	15.131	28.348	1.00	46.19	B
ATOM	4746	C	ARG	B	245	17.233	11.102	33.486	1.00	40.09	B
ATOM	4747	O	ARG	B	245	17.574	10.297	34.352	1.00	40.05	B
ATOM	4748	N	ARG	B	246	16.133	11.840	33.560	1.00	39.85	B
ATOM	4749	CA	ARG	B	246	15.239	11.808	34.707	1.00	40.96	B
ATOM	4750	CB	ARG	B	246	14.755	13.227	34.984	1.00	43.17	B
ATOM	4751	CG	ARG	B	246	15.880	14.252	35.113	1.00	46.06	B
ATOM	4752	CD	ARG	B	246	16.443	14.295	36.529	1.00	47.96	B
ATOM	4753	NE	ARG	B	246	15.374	14.318	37.524	1.00	49.96	B
ATOM	4754	CZ	ARG	B	246	14.316	15.126	37.477	1.00	50.99	B
ATOM	4755	NH1	ARG	B	246	14.169	15.992	36.481	1.00	51.52	B
ATOM	4756	NH2	ARG	B	246	13.396	15.067	38.430	1.00	52.32	B
ATOM	4757	C	ARG	B	246	14.022	10.889	34.566	1.00	40.13	B
ATOM	4758	O	ARG	B	246	13.384	10.536	35.560	1.00	39.22	B
ATOM	4759	N	VAL	B	247	13.695	10.532	33.327	1.00	38.72	B
ATOM	4760	CA	VAL	B	247	12.553	9.675	33.018	1.00	36.88	B
ATOM	4761	CB	VAL	B	247	12.061	9.942	31.585	1.00	37.39	B
ATOM	4762	CG1	VAL	B	247	10.930	8.991	31.216	1.00	36.97	B
ATOM	4763	CG2	VAL	B	247	11.624	11.391	31.462	1.00	37.68	B
ATOM	4764	C	VAL	B	247	12.962	8.218	33.133	1.00	35.57	B
ATOM	4765	O	VAL	B	247	12.125	7.334	33.308	1.00	36.36	B

Figure 1 (continued 48)

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ATOM	4766	N	LEU	B	248	14.260	7.974	33.019	1.00	34.36	B
ATOM	4767	CA	LEU	B	248	14.797	6.627	33.124	1.00	34.03	B
ATOM	4768	CB	LEU	B	248	16.296	6.521	32.855	1.00	33.66	B
ATOM	4769	CG	LEU	B	248	16.785	7.109	31.493	1.00	33.85	B
ATOM	4770	CD1	LEU	B	248	16.285	6.813	31.398	1.00	34.48	B
ATOM	4771	CD2	LEU	B	248	16.017	6.403	30.386	1.00	33.89	B
ATOM	4772	C	LEU	B	248	14.564	6.083	34.525	1.00	34.01	B
ATOM	4773	O	LEU	B	248	14.860	6.756	35.519	1.00	32.99	B
ATOM	4774	N	PRO	B	249	14.038	4.851	34.622	1.00	33.37	B
ATOM	4775	CD	PRO	B	249	13.707	3.936	33.514	1.00	32.25	B
ATOM	4776	CA	PRO	B	249	13.776	4.221	35.921	1.00	33.57	B
ATOM	4777	CB	PRO	B	249	13.565	2.751	35.546	1.00	32.82	B
ATOM	4778	CG	PRO	B	249	12.921	2.845	34.210	1.00	32.30	B
ATOM	4779	C	PRO	B	249	14.965	4.423	36.875	1.00	33.81	B
ATOM	4780	O	PRO	B	249	16.113	4.182	36.514	1.00	31.74	B
ATOM	4781	N	LYS	B	250	14.672	4.869	38.091	1.00	36.30	B
ATOM	4782	CA	LYS	B	250	15.695	5.128	39.102	1.00	39.83	B
ATOM	4783	CB	LYS	B	250	15.024	5.653	40.370	1.00	41.65	B
ATOM	4784	CG	LYS	B	250	13.622	6.224	40.144	1.00	44.53	B
ATOM	4785	CD	LYS	B	250	12.980	6.637	41.466	1.00	46.40	B
ATOM	4786	CE	LYS	B	250	11.562	7.139	41.267	1.00	47.75	B
ATOM	4787	NZ	LYS	B	250	10.957	7.618	42.538	1.00	48.54	B
ATOM	4788	C	LYS	B	250	16.562	3.912	39.454	1.00	40.80	B
ATOM	4789	O	LYS	B	250	17.773	3.915	39.240	1.00	42.14	B
ATOM	4790	N	ASN	B	251	15.944	2.881	40.016	1.00	40.30	B
ATOM	4791	CA	ASN	B	251	16.687	1.686	40.388	1.00	41.84	B
ATOM	4792	CB	ASN	B	251	16.907	1.661	41.899	1.00	43.14	B
ATOM	4793	CG	ASN	B	251	17.875	2.734	42.365	1.00	44.47	B
ATOM	4794	OD1	ASN	B	251	17.623	3.421	43.353	1.00	45.51	B
ATOM	4795	ND2	ASN	B	251	18.996	2.873	41.662	1.00	45.61	B
ATOM	4796	C	ASN	B	251	15.976	0.413	39.942	1.00	41.06	B
ATOM	4797	O	ASN	B	251	15.388	-0.302	40.754	1.00	40.34	B
ATOM	4798	N	PRO	B	252	16.020	0.121	38.634	1.00	40.93	B
ATOM	4799	CD	PRO	B	252	16.646	0.951	37.592	1.00	40.87	B
ATOM	4800	CA	PRO	B	252	15.384	-1.069	38.051	1.00	40.56	B
ATOM	4801	CB	PRO	B	252	15.505	-0.839	36.539	1.00	40.95	B
ATOM	4802	CG	PRO	B	252	15.797	0.628	36.393	1.00	41.84	B
ATOM	4803	C	PRO	B	252	16.144	-2.323	38.481	1.00	40.59	B
ATOM	4804	O	PRO	B	252	16.811	-2.953	37.666	1.00	41.49	B
ATOM	4805	N	ASP	B	253	16.024	-2.681	39.754	1.00	39.23	B
ATOM	4806	CA	ASP	B	253	16.725	-3.833	40.318	1.00	38.72	B
ATOM	4807	CB	ASP	B	253	16.316	-4.011	41.799	1.00	40.83	B
ATOM	4808	CG	ASP	B	253	14.803	-4.237	41.995	1.00	42.90	B
ATOM	4809	OD1	ASP	B	253	13.992	-3.318	41.739	1.00	44.02	B
ATOM	4810	OD2	ASP	B	253	14.413	-5.347	42.423	1.00	44.75	B
ATOM	4811	C	ASP	B	253	16.616	-5.183	39.585	1.00	36.72	B
ATOM	4812	O	ASP	B	253	17.601	-5.922	39.478	1.00	36.03	B
ATOM	4813	N	LYS	B	254	15.432	-5.484	39.066	1.00	32.67	B
ATOM	4814	CA	LYS	B	254	15.164	-6.751	38.403	1.00	30.08	B
ATOM	4815	CB	LYS	B	254	13.688	-7.106	38.593	1.00	28.89	B
ATOM	4816	CG	LYS	B	254	13.194	-7.092	40.049	1.00	29.78	B
ATOM	4817	CD	LYS	B	254	11.661	-7.160	40.098	1.00	28.23	B
ATOM	4818	CE	LYS	B	254	11.120	-7.160	41.515	1.00	33.00	B
ATOM	4819	NZ	LYS	B	254	11.584	-5.968	42.297	1.00	33.49	B
ATOM	4820	C	LYS	B	254	15.489	-6.736	36.912	1.00	29.93	B
ATOM	4821	O	LYS	B	254	14.811	-6.060	36.135	1.00	30.36	B
ATOM	4822	N	HIS	B	255	16.495	-7.501	36.519	1.00	27.24	B
ATOM	4823	CA	HIS	B	255	16.897	-7.564	35.118	1.00	26.91	B
ATOM	4824	CB	HIS	B	255	18.402	-7.339	34.966	1.00	30.35	B
ATOM	4825	CG	HIS	B	255	18.876	-6.000	35.429	1.00	33.70	B
ATOM	4826	CD2	HIS	B	255	20.129	-5.522	35.617	1.00	34.19	B
ATOM	4827	ND1	HIS	B	255	18.021	-4.950	35.695	1.00	35.10	B
ATOM	4828	CE1	HIS	B	255	18.730	-3.882	36.025	1.00	35.55	B
ATOM	4829	NE2	HIS	B	255	20.011	-4.204	35.986	1.00	34.99	B
ATOM	4830	C	HIS	B	255	16.587	-8.885	34.453	1.00	24.52	B
ATOM	4831	O	HIS	B	255	16.979	-9.935	34.936	1.00	23.10	B
ATOM	4832	N	LEU	B	256	15.923	-8.824	33.107	1.00	22.74	B
ATOM	4833	CA	LEU	B	256	15.606	-10.014	32.551	1.00	21.40	B
ATOM	4834	CB	LEU	B	256	14.080	-10.157	32.461	1.00	23.90	B
ATOM	4835	CG	LEU	B	256	13.435	-11.154	31.508	1.00	24.90	B
ATOM	4836	CD1	LEU	B	256	12.064	-11.555	32.033	1.00	26.89	B
ATOM	4837	CD2	LEU	B	256	13.322	-10.514	30.136	1.00	23.55	B
ATOM	4838	C	LEU	B	256	16.210	-9.867	31.154	1.00	19.61	B
ATOM	4839	O	LEU	B	256	16.191	-8.768	30.581	1.00	18.29	B
ATOM	4840	N	GLU	B	257	16.774	-10.955	30.641	1.00	18.37	B
ATOM	4841	CA	GLU	B	257	17.329	-10.973	29.287	1.00	18.54	B
ATOM	4842	CB	GLU	B	257	18.848	-11.229	29.318	1.00	21.51	B
ATOM	4843	CG	GLU	B	257	19.681	-10.093	29.921	1.00	27.65	B
ATOM	4844	CD	GLU	B	257	19.758	-10.132	31.460	1.00	31.19	B
ATOM	4845	OE1	GLU	B	257	19.940	-11.236	32.023	1.00	33.27	B
ATOM	4846	OE2	GLU	B	257	19.664	-9.056	32.108	1.00	32.03	B
ATOM	4847	C	GLU	B	257	16.616	-12.085	28.510	1.00	17.69	B
ATOM	4848	O	GLU	B	257	16.374	-13.182	29.042	1.00	18.75	B
ATOM	4849	N	ALA	B	258	16.262	-11.808	27.256	1.00	17.24	B
ATOM	4850	CA	ALA	B	258	15.558	-12.786	26.423	1.00	18.43	B
ATOM	4851	CB	ALA	B	258	14.079	-12.680	26.654	1.00	22.18	B
ATOM	4852	CG	ALA	B	258	15.840	-12.507	24.966	1.00	19.20	B
ATOM	4853	CD	ALA	B	258	16.180	-11.370	24.609	1.00	19.32	B
ATOM	4854	CE	GLY	B	259	15.713	-13.539	24.130	1.00	18.97	B
ATOM	4855	N	GLY	B	259	15.917	-13.346	22.700	1.00	18.87	B
ATOM	4856	CA	GLY	B	259	14.894	-12.358	23.161	1.00	19.04	B
ATOM	4857	CB	GLY	B	259	13.693	-12.468	22.453	1.00	18.24	B
ATOM	4858	N	CYS	B	260	15.356	-11.389	21.375	1.00	17.25	B
ATOM	4859	CA	CYS	B	260	14.439	-10.387	20.846	1.00	18.30	B
ATOM	4860	CB	CYS	B	260	15.216	-9.341	20.048	1.00	17.26	B
ATOM	4861	SG	CYS	B	260	14.169	-7.950	19.540	1.00	23.04	B
ATOM	4862	C	CYS	B	260	13.335	-10.980	19.981	1.00	17.67	B
ATOM	4863	O	CYS	B	260	12.164	-10.678	20.188	1.00	18.38	B
ATOM	4864	N	ASP	B	261	13.694	-11.811	19.006	1.00	18.04	B
ATOM	4865	CA	ASP	B	261	12.666	-12.364	18.140	1.00	18.32	B

Figure 1 (continued 49)

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ATOM	4866	CB	ASP	B	261	13.290	-13.046	16.919	1.00	21.68	B
ATOM	4867	CG	ASP	B	261	12.334	-13.065	15.738	1.00	24.40	B
ATOM	4868	OD1	ASP	B	261	11.951	-14.160	15.306	1.00	27.81	B
ATOM	4869	OD2	ASP	B	261	11.957	-11.968	15.252	1.00	22.15	B
ATOM	4870	O	ASP	B	261	11.685	-13.311	18.828	1.00	16.90	B
ATOM	4871	C	ASP	B	261	10.480	-13.263	18.540	1.00	17.30	B
ATOM	4872	N	LEU	B	262	12.154	-14.159	19.737	1.00	14.56	B
ATOM	4873	CA	LEU	B	262	11.191	-15.037	20.412	1.00	17.35	B
ATOM	4874	CB	LEU	B	262	11.872	-16.053	21.329	1.00	19.61	B
ATOM	4875	CG	LEU	B	262	12.472	-17.269	20.638	1.00	19.99	B
ATOM	4876	CD1	LEU	B	262	13.259	-18.057	21.656	1.00	21.84	B
ATOM	4877	CD2	LEU	B	262	11.395	-18.129	19.939	1.00	21.69	B
ATOM	4878	C	LEU	B	262	10.248	-14.170	21.243	1.00	15.38	B
ATOM	4879	N	LEU	B	262	9.065	-14.433	21.311	1.00	15.79	B
ATOM	4880	CA	LEU	B	263	10.780	-13.136	21.892	1.00	15.25	B
ATOM	4881	CB	LEU	B	263	9.923	-12.288	22.713	1.00	16.20	B
ATOM	4882	CG	LEU	B	263	10.795	-11.293	23.487	1.00	18.03	B
ATOM	4883	CD1	LEU	B	263	10.111	-10.421	24.532	1.00	21.36	B
ATOM	4884	CD2	LEU	B	263	9.540	-11.366	25.608	1.00	21.04	B
ATOM	4885	O	LEU	B	263	11.103	-9.396	25.155	1.00	22.83	B
ATOM	4886	C	LEU	B	263	8.916	-11.546	21.826	1.00	16.77	B
ATOM	4887	N	LYS	B	263	7.735	-11.457	22.133	1.00	15.34	B
ATOM	4888	CA	LYS	B	264	9.395	-11.034	20.711	1.00	16.41	B
ATOM	4889	CB	LYS	B	264	8.525	-10.302	19.806	1.00	16.03	B
ATOM	4890	CG	LYS	B	264	9.335	-9.738	18.636	1.00	18.07	B
ATOM	4891	CD1	LYS	B	264	8.475	-9.099	17.595	1.00	22.20	B
ATOM	4892	CD2	LYS	B	264	9.281	-8.250	16.610	1.00	26.37	B
ATOM	4893	C	LYS	B	264	10.346	-9.023	15.870	1.00	28.03	B
ATOM	4894	NZ	LYS	B	264	11.318	-8.076	15.214	1.00	31.01	B
ATOM	4895	O	LYS	B	264	7.412	-11.191	19.262	1.00	15.79	B
ATOM	4896	C	LYS	B	264	6.236	-10.796	19.245	1.00	14.64	B
ATOM	4897	N	GLN	B	265	7.784	-12.391	18.817	1.00	15.72	B
ATOM	4898	CA	GLN	B	265	6.779	-13.286	18.244	1.00	16.84	B
ATOM	4899	CB	GLN	B	265	7.435	-14.519	17.598	1.00	17.09	B
ATOM	4900	CG	GLN	B	265	8.320	-14.204	16.357	1.00	18.42	B
ATOM	4901	CD1	GLN	B	265	7.782	-13.068	15.479	1.00	22.54	B
ATOM	4902	OE1	GLN	B	265	6.570	-12.890	15.303	1.00	26.47	B
ATOM	4903	NE2	GLN	B	265	8.704	-12.294	14.913	1.00	25.44	B
ATOM	4904	C	GLN	B	265	5.753	-13.721	19.293	1.00	14.97	B
ATOM	4905	O	GLN	B	265	4.572	-13.896	18.984	1.00	15.81	B
ATOM	4906	N	ALA	B	266	6.185	-13.892	20.535	1.00	15.47	B
ATOM	4907	CA	ALA	B	266	5.255	-14.301	21.598	1.00	14.14	B
ATOM	4908	CB	ALA	B	266	6.022	-14.664	22.883	1.00	15.40	B
ATOM	4909	C	ALA	B	266	4.283	-13.174	21.879	1.00	15.29	B
ATOM	4910	N	ALA	B	266	3.083	-13.405	22.019	1.00	13.58	B
ATOM	4911	O	PHE	B	267	4.807	-11.951	21.974	1.00	13.20	B
ATOM	4912	CA	PHE	B	267	3.921	-10.801	22.218	1.00	13.52	B
ATOM	4913	CB	PHE	B	267	4.744	-9.513	22.439	1.00	13.38	B
ATOM	4914	CG	PHE	B	267	5.198	-9.317	23.868	1.00	13.24	B
ATOM	4915	CD1	PHE	B	267	4.271	-9.194	24.912	1.00	14.43	B
ATOM	4916	CD2	PHE	B	267	6.565	-9.244	24.169	1.00	14.23	B
ATOM	4917	CE1	PHE	B	267	4.694	-8.992	26.240	1.00	16.33	B
ATOM	4918	CE2	PHE	B	267	6.986	-9.048	25.487	1.00	16.29	B
ATOM	4919	C	PHE	B	267	6.051	-8.920	26.516	1.00	15.41	B
ATOM	4920	N	PHE	B	267	2.960	-10.609	21.038	1.00	14.30	B
ATOM	4921	O	PHE	B	267	1.788	-10.261	21.248	1.00	14.42	B
ATOM	4922	CA	ALA	B	268	3.446	-10.818	19.813	1.00	14.41	B
ATOM	4923	CB	ALA	B	268	2.630	-10.628	18.615	1.00	15.14	B
ATOM	4924	C	ALA	B	268	3.504	-10.794	17.379	1.00	14.71	B
ATOM	4925	N	ALA	B	268	1.480	-11.633	18.606	1.00	14.93	B
ATOM	4926	O	ALA	B	268	0.329	-11.286	18.247	1.00	14.13	B
ATOM	4927	CA	ARG	B	269	1.757	-12.880	19.008	1.00	13.12	B
ATOM	4928	CB	ARG	B	269	0.671	-13.840	19.015	1.00	13.27	B
ATOM	4929	CG	ARG	B	269	1.214	-15.269	19.154	1.00	14.61	B
ATOM	4930	CD	ARG	B	269	1.831	-15.845	17.872	1.00	13.63	B
ATOM	4931	NE	ARG	B	269	2.204	-17.358	18.026	1.00	13.98	B
ATOM	4932	CZ	ARG	B	269	3.118	-17.555	19.133	1.00	13.12	B
ATOM	4933	NH1	ARG	B	269	4.448	-17.518	19.033	1.00	15.76	B
ATOM	4934	NH2	ARG	B	269	5.034	-17.313	17.853	1.00	14.76	B
ATOM	4935	C	ARG	B	269	5.201	-17.683	20.114	1.00	14.02	B
ATOM	4936	N	ARG	B	269	-0.324	-13.530	20.153	1.00	14.05	B
ATOM	4937	CA	ALA	B	270	-1.546	-13.617	19.952	1.00	14.17	B
ATOM	4938	CB	ALA	B	270	0.191	-13.167	21.338	1.00	13.89	B
ATOM	4939	C	ALA	B	270	-0.687	-12.886	22.471	1.00	14.30	B
ATOM	4940	N	ALA	B	270	0.141	-12.603	23.735	1.00	13.36	B
ATOM	4941	O	ALA	B	270	-1.568	-11.682	22.159	1.00	13.96	B
ATOM	4942	CA	ALA	B	271	-2.748	-11.645	22.542	1.00	15.55	B
ATOM	4943	CB	ALA	B	271	-1.002	-10.720	21.438	1.00	14.27	B
ATOM	4944	C	ALA	B	271	-1.726	-9.500	21.096	1.00	13.67	B
ATOM	4945	N	ALA	B	271	-0.836	-8.599	20.291	1.00	15.13	B
ATOM	4946	O	ALA	B	271	-3.002	-9.795	20.333	1.00	15.03	B
ATOM	4947	CA	ILE	B	272	-3.972	-9.041	20.421	1.00	15.64	B
ATOM	4948	CB	ILE	B	272	-3.016	-10.898	19.595	1.00	14.65	B
ATOM	4949	C	ILE	B	272	-4.196	-11.249	18.821	1.00	15.22	B
ATOM	4950	N	ILE	B	272	-3.974	-12.585	18.079	1.00	13.73	B
ATOM	4951	CG2	ILE	B	272	-5.242	-13.018	17.334	1.00	15.77	B
ATOM	4952	CG1	ILE	B	272	-2.854	-12.439	17.060	1.00	15.68	B
ATOM	4953	CD1	ILE	B	272	-2.364	-13.817	16.555	1.00	16.71	B
ATOM	4954	C	ILE	B	272	-5.430	-11.343	19.725	1.00	16.21	B
ATOM	4955	N	ILE	B	272	-6.524	-10.941	19.311	1.00	16.96	B
ATOM	4956	O	LEU	B	273	-5.277	-11.870	20.949	1.00	16.13	B
ATOM	4957	CA	LEU	B	273	-6.425	-11.991	21.858	1.00	15.61	B
ATOM	4958	CB	LEU	B	273	-6.508	-13.415	22.449	1.00	16.11	B
ATOM	4959	CG	LEU	B	273	-6.563	-14.492	21.330	1.00	16.18	B
ATOM	4960	CD1	LEU	B	273	-6.548	-15.891	21.960	1.00	16.52	B
ATOM	4961	CD2	LEU	B	273	-7.847	-14.316	20.469	1.00	18.42	B
ATOM	4962	C	LEU	B	273	-6.473	-10.946	22.968	1.00	17.30	B
ATOM	4963	N	LEU	B	273	-7.106	-11.158	23.997	1.00	17.88	B
ATOM	4964	O	SER	B	274	-5.811	-9.809	22.742	1.00	17.24	B
ATOM	4965	CA	SER	B	274	-5.863	-8.708	23.702	1.00	18.02	B

Figure 1 (continued 50)

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ATOM	4966	CB	SER	B	274	-4.556	-7.906	23.686	1.00	17.37	B
ATOM	4967	OG	SER	B	274	-4.390	-7.180	22.474	1.00	17.38	B
ATOM	4968	C	SER	B	274	-7.033	-7.796	23.318	1.00	17.71	B
ATOM	4969	O	SER	B	274	-7.542	-7.858	22.189	1.00	17.27	B
ATOM	4970	N	ASN	B	275	-7.464	-6.965	24.260	1.00	17.56	B
ATOM	4971	CA	ASN	B	275	-8.550	-6.014	24.026	1.00	18.55	B
ATOM	4972	CB	ASN	B	275	-8.705	-5.145	25.269	1.00	17.80	B
ATOM	4973	CG	ASN	B	275	-9.904	-4.223	25.180	1.00	19.42	B
ATOM	4974	OD1	ASN	B	275	-9.934	-3.339	24.331	1.00	19.77	B
ATOM	4975	ND2	ASN	B	275	-10.898	-4.431	26.063	1.00	22.03	B
ATOM	4976	C	ASN	B	275	-8.184	-5.166	22.792	1.00	20.76	B
ATOM	4977	O	ASN	B	275	-7.090	-4.585	22.723	1.00	17.98	B
ATOM	4978	N	GLU	B	276	-9.091	-5.093	21.816	1.00	21.76	B
ATOM	4979	CA	GLU	B	276	-8.779	-4.365	20.591	1.00	23.72	B
ATOM	4980	CB	GLU	B	276	-9.897	-4.556	19.554	1.00	25.43	B
ATOM	4981	CG	GLU	B	276	-9.852	-5.932	18.891	1.00	29.37	B
ATOM	4982	CD	GLU	B	276	-11.021	-6.196	17.960	1.00	32.27	B
ATOM	4983	OE1	GLU	B	276	-11.600	-5.217	17.442	1.00	33.37	B
ATOM	4984	OE2	GLU	B	276	-11.348	-7.390	17.745	1.00	32.65	B
ATOM	4985	C	GLU	B	276	-8.481	-2.888	20.782	1.00	23.01	B
ATOM	4986	O	GLU	B	276	-7.749	-2.292	19.986	1.00	23.94	B
ATOM	4987	N	LYS	B	277	-9.034	-2.310	21.837	1.00	23.05	B
ATOM	4988	CA	LYS	B	277	-8.810	-0.910	22.113	1.00	23.82	B
ATOM	4989	CB	LYS	B	277	-10.085	-0.230	22.638	1.00	25.13	B
ATOM	4990	CG	LYS	B	277	-9.852	1.262	22.949	1.00	28.98	B
ATOM	4991	CD	LYS	B	277	-11.084	2.016	23.463	1.00	31.73	B
ATOM	4992	CE	LYS	B	277	-10.744	3.512	23.598	1.00	33.68	B
ATOM	4993	NZ	LYS	B	277	-11.577	4.222	24.623	1.00	35.35	B
ATOM	4994	C	LYS	B	277	-7.681	-0.655	23.104	1.00	23.58	B
ATOM	4995	O	LYS	B	277	-6.790	0.162	22.825	1.00	23.95	B
ATOM	4996	N	PHE	B	278	-7.702	-1.352	24.244	1.00	21.16	B
ATOM	4997	CA	PHE	B	278	-6.698	-1.155	25.300	1.00	20.62	B
ATOM	4998	CB	PHE	B	278	-7.318	-1.432	26.663	1.00	21.99	B
ATOM	4999	CG	PHE	B	278	-8.431	-0.459	27.021	1.00	26.60	B
ATOM	5000	CD1	PHE	B	278	-8.142	0.882	27.268	1.00	29.14	B
ATOM	5001	CD2	PHE	B	278	-9.760	-0.869	27.021	1.00	28.88	B
ATOM	5002	CE1	PHE	B	278	-9.177	1.816	27.508	1.00	30.11	B
ATOM	5003	CE2	PHE	B	278	-10.795	0.052	27.258	1.00	30.65	B
ATOM	5004	CZ	PHE	B	278	-10.496	1.391	27.500	1.00	30.56	B
ATOM	5005	C	PHE	B	278	-5.403	-1.957	25.131	1.00	19.25	B
ATOM	5006	O	PHE	B	278	-4.356	-1.582	25.677	1.00	18.94	B
ATOM	5007	N	ARG	B	279	-5.484	-3.045	24.371	1.00	19.60	B
ATOM	5008	CA	ARG	B	279	-4.307	-3.865	24.050	1.00	18.45	B
ATOM	5009	CB	ARG	B	279	-3.404	-3.067	23.088	1.00	19.81	B
ATOM	5010	CG	ARG	B	279	-4.078	-2.674	21.767	1.00	19.94	B
ATOM	5011	CD	ARG	B	279	-4.097	-3.843	20.776	1.00	21.13	B
ATOM	5012	NE	ARG	B	279	-2.777	-3.988	20.175	1.00	23.76	B
ATOM	5013	CZ	ARG	B	279	-2.423	-4.973	19.365	1.00	22.43	B
ATOM	5014	NH1	ARG	B	279	-3.297	-5.921	19.058	1.00	25.01	B
ATOM	5015	NH2	ARG	B	279	-1.202	-4.987	18.838	1.00	23.93	B
ATOM	5016	C	ARG	B	279	-3.460	-4.360	25.210	1.00	18.23	B
ATOM	5017	O	ARG	B	279	-2.261	-4.590	25.046	1.00	16.99	B
ATOM	5018	N	GLY	B	280	-4.062	-4.589	26.365	1.00	16.92	B
ATOM	5019	CA	GLY	B	280	-3.260	-5.011	27.491	1.00	15.52	B
ATOM	5020	C	GLY	B	280	-2.864	-6.477	27.534	1.00	14.43	B
ATOM	5021	O	GLY	B	280	-3.652	-7.360	27.199	1.00	15.18	B
ATOM	5022	N	VAL	B	281	-1.623	-6.709	27.942	1.00	15.08	B
ATOM	5023	CA	VAL	B	281	-1.104	-8.062	28.125	1.00	14.23	B
ATOM	5024	CB	VAL	B	281	-0.046	-8.473	27.057	1.00	12.60	B
ATOM	5025	CG1	VAL	B	281	-0.707	-8.654	25.727	1.00	17.31	B
ATOM	5026	CG2	VAL	B	281	1.061	-7.440	26.981	1.00	15.23	B
ATOM	5027	C	VAL	B	281	-0.450	-8.059	29.497	1.00	13.94	B
ATOM	5028	O	VAL	B	281	-0.049	-7.000	30.034	1.00	14.27	B
ATOM	5029	N	ARG	B	282	-0.387	-9.241	30.091	1.00	12.68	B
ATOM	5030	CA	ARG	B	282	0.202	-9.381	31.405	1.00	14.01	B
ATOM	5031	CB	ARG	B	282	-0.753	-10.142	32.337	1.00	18.49	B
ATOM	5032	CG	ARG	B	282	-1.999	-9.373	32.712	1.00	25.67	B
ATOM	5033	CD	ARG	B	282	-2.770	-10.154	33.784	1.00	31.13	B
ATOM	5034	NE	ARG	B	282	-3.601	-9.274	34.606	1.00	36.93	B
ATOM	5035	CZ	ARG	B	282	-3.765	-9.449	35.908	1.00	38.95	B
ATOM	5036	NH1	ARG	B	282	-3.154	-10.470	36.510	1.00	41.34	B
ATOM	5037	NH2	ARG	B	282	-4.511	-8.605	36.615	1.00	42.07	B
ATOM	5038	C	ARG	B	282	1.489	-10.168	31.273	1.00	13.94	B
ATOM	5039	O	ARG	B	282	1.568	-11.118	30.483	1.00	13.78	B
ATOM	5040	N	LEU	B	283	2.503	-9.736	32.016	1.00	11.77	B
ATOM	5041	CA	LEU	B	283	3.784	-10.427	32.050	1.00	12.94	B
ATOM	5042	CB	LEU	B	283	4.931	-9.460	31.806	1.00	13.78	B
ATOM	5043	CG	LEU	B	283	5.246	-9.059	30.376	1.00	16.55	B
ATOM	5044	CD1	LEU	B	283	4.078	-8.291	29.772	1.00	18.52	B
ATOM	5045	CD2	LEU	B	283	6.512	-8.199	30.417	1.00	15.82	B
ATOM	5046	C	LEU	B	283	3.989	-10.979	33.454	1.00	13.65	B
ATOM	5047	O	LEU	B	283	3.832	-10.232	34.422	1.00	15.26	B
ATOM	5048	N	TYR	B	284	4.281	-12.271	33.584	1.00	13.05	B
ATOM	5049	CA	TYR	B	284	4.580	-12.809	34.913	1.00	13.63	B
ATOM	5050	CB	TYR	B	284	3.686	-14.004	35.283	1.00	13.56	B
ATOM	5051	CG	TYR	B	284	3.808	-14.302	36.781	1.00	18.42	B
ATOM	5052	CD1	TYR	B	284	2.898	-13.778	37.698	1.00	20.54	B
ATOM	5053	CE1	TYR	B	284	3.069	-13.971	39.101	1.00	22.11	B
ATOM	5054	CD2	TYR	B	284	4.890	-15.024	37.260	1.00	19.69	B
ATOM	5055	CE2	TYR	B	284	5.088	-15.221	38.628	1.00	20.37	B
ATOM	5056	CZ	TYR	B	284	4.175	-14.694	39.544	1.00	22.54	B
ATOM	5057	OH	TYR	B	284	4.412	-14.897	40.899	1.00	21.81	B
ATOM	5058	C	TYR	B	284	6.027	-13.271	34.818	1.00	12.58	B
ATOM	5059	O	TYR	B	284	6.357	-14.144	34.036	1.00	13.78	B
ATOM	5060	N	VAL	B	285	6.898	-12.675	35.635	1.00	12.36	B
ATOM	5061	CA	VAL	B	285	8.306	-12.990	35.601	1.00	13.80	B
ATOM	5062	CB	VAL	B	285	9.106	-11.669	35.724	1.00	16.86	B
ATOM	5063	CG1	VAL	B	285	10.576	-11.922	35.640	1.00	20.79	B
ATOM	5064	CG2	VAL	B	285	8.675	-10.718	34.599	1.00	19.51	B
ATOM	5065	C	VAL	B	285	8.656	-13.928	36.761	1.00	12.81	B

Figure 1 (continued 51)

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ATOM	5066	O	VAL	B	285	8.313	-13.643	37.889	1.00	14.44	B
ATOM	5067	N	SER	B	286	9.318	-15.036	36.464	1.00	13.79	B
ATOM	5068	CA	SER	B	286	9.730	-15.996	37.493	1.00	14.29	B
ATOM	5069	CB	SER	B	286	8.716	-17.148	37.609	1.00	14.83	B
ATOM	5070	OG	SER	B	286	8.623	-17.928	36.439	1.00	17.73	B
ATOM	5071	C	SER	B	286	11.145	-16.492	37.139	1.00	14.68	B
ATOM	5072	O	SER	B	286	11.712	-16.316	36.103	1.00	14.34	B
ATOM	5073	N	GLU	B	287	11.732	-17.732	37.971	1.00	15.06	B
ATOM	5074	CA	GLU	B	287	13.112	-17.732	37.692	1.00	16.29	B
ATOM	5075	CB	GLU	B	287	13.621	-18.691	38.764	1.00	16.48	B
ATOM	5076	CG	GLU	B	287	15.094	-19.065	38.591	1.00	20.87	B
ATOM	5077	CD	GLU	B	287	15.613	-19.806	39.813	1.00	24.94	B
ATOM	5078	OE1	GLU	B	287	15.225	-20.975	40.008	1.00	28.92	B
ATOM	5079	OE2	GLU	B	287	16.400	-19.205	40.580	1.00	32.02	B
ATOM	5080	C	GLU	B	287	13.278	-18.314	36.296	1.00	15.72	B
ATOM	5081	O	GLU	B	287	12.644	-19.303	35.921	1.00	15.04	B
ATOM	5082	N	ASN	B	288	14.134	-17.655	35.518	1.00	14.89	B
ATOM	5083	CA	ASN	B	288	14.386	-18.021	34.127	1.00	15.81	B
ATOM	5084	CB	ASN	B	288	15.363	-19.200	34.049	1.00	17.29	B
ATOM	5085	CG	ASN	B	288	16.736	-18.812	34.607	1.00	19.00	B
ATOM	5086	OD1	ASN	B	288	17.095	-17.642	34.575	1.00	18.60	B
ATOM	5087	ND2	ASN	B	288	17.496	-19.779	35.122	1.00	22.68	B
ATOM	5088	C	ASN	B	288	13.146	-18.280	33.271	1.00	14.61	B
ATOM	5089	O	ASN	B	288	13.196	-19.064	32.325	1.00	15.72	B
ATOM	5090	N	GLN	B	289	12.047	-17.592	33.589	1.00	12.93	B
ATOM	5091	CA	GLN	B	289	10.834	-17.771	32.806	1.00	13.30	B
ATOM	5092	CB	GLN	B	289	9.979	-18.907	33.380	1.00	14.55	B
ATOM	5093	CG	GLN	B	289	8.664	-19.147	32.605	1.00	18.51	B
ATOM	5094	CD	GLN	B	289	7.737	-20.171	33.274	1.00	20.32	B
ATOM	5095	OE1	GLN	B	289	6.714	-19.820	33.912	1.00	24.66	B
ATOM	5096	NE2	GLN	B	289	8.084	-21.430	33.128	1.00	20.90	B
ATOM	5097	C	GLN	B	289	9.950	-16.543	32.706	1.00	13.31	B
ATOM	5098	O	GLN	B	289	9.796	-15.783	33.648	1.00	11.95	B
ATOM	5099	N	LEU	B	290	9.382	-16.347	31.513	1.00	12.64	B
ATOM	5100	CA	LEU	B	290	8.438	-15.253	31.315	1.00	13.02	B
ATOM	5101	CB	LEU	B	290	8.990	-14.220	30.294	1.00	14.05	B
ATOM	5102	CG	LEU	B	290	7.961	-13.160	29.861	1.00	15.71	B
ATOM	5103	CD1	LEU	B	290	7.482	-12.331	31.070	1.00	17.91	B
ATOM	5104	CD2	LEU	B	290	8.586	-12.240	28.816	1.00	17.17	B
ATOM	5105	C	LEU	B	290	7.155	-15.864	30.777	1.00	12.56	B
ATOM	5106	O	LEU	B	290	7.201	-16.657	29.836	1.00	14.23	B
ATOM	5107	N	LYS	B	291	6.022	-15.521	31.391	1.00	12.00	B
ATOM	5108	CA	LYS	B	291	4.723	-15.991	30.909	1.00	12.78	B
ATOM	5109	CB	LYS	B	291	3.958	-16.744	32.014	1.00	14.55	B
ATOM	5110	CG	LYS	B	291	2.521	-17.061	31.604	1.00	17.33	B
ATOM	5111	CD	LYS	B	291	1.794	-17.803	32.734	1.00	23.96	B
ATOM	5112	CE	LYS	B	291	0.313	-17.910	32.428	1.00	28.19	B
ATOM	5113	NZ	LYS	B	291	-0.532	-18.367	33.595	1.00	33.90	B
ATOM	5114	C	LYS	B	291	3.975	-14.725	30.480	1.00	13.62	B
ATOM	5115	O	LYS	B	291	3.869	-13.757	31.243	1.00	15.74	B
ATOM	5116	N	ILE	B	292	3.487	-14.708	29.241	1.00	11.68	B
ATOM	5117	CA	ILE	B	292	2.736	-13.572	28.712	1.00	12.10	B
ATOM	5118	CB	ILE	B	292	3.318	-13.132	27.329	1.00	12.34	B
ATOM	5119	CG2	ILE	B	292	2.448	-12.013	26.690	1.00	14.58	B
ATOM	5120	CG1	ILE	B	292	4.739	-12.646	27.525	1.00	15.22	B
ATOM	5121	CD1	ILE	B	292	5.529	-12.532	26.240	1.00	17.04	B
ATOM	5122	C	ILE	B	292	1.303	-14.048	28.511	1.00	12.60	B
ATOM	5123	O	ILE	B	292	1.075	-15.065	27.844	1.00	13.06	B
ATOM	5124	N	THR	B	293	0.340	-13.316	29.072	1.00	12.37	B
ATOM	5125	CA	THR	B	293	-1.050	-13.703	28.891	1.00	13.44	B
ATOM	5126	CB	THR	B	293	-1.699	-14.182	30.200	1.00	14.23	B
ATOM	5127	OG1	THR	B	293	-1.641	-13.160	31.179	1.00	18.90	B
ATOM	5128	CG2	THR	B	293	-0.947	-15.366	30.766	1.00	15.88	B
ATOM	5129	C	THR	B	293	-1.832	-12.525	28.372	1.00	14.34	B
ATOM	5130	O	THR	B	293	-1.471	-11.362	28.600	1.00	13.84	B
ATOM	5131	N	ALA	B	294	-2.883	-12.837	27.634	1.00	12.99	B
ATOM	5132	CA	ALA	B	294	-3.746	-11.800	27.101	1.00	14.01	B
ATOM	5133	CB	ALA	B	294	-5.325	-11.469	25.644	1.00	15.00	B
ATOM	5134	C	ALA	B	294	-5.164	-12.333	27.116	1.00	15.21	B
ATOM	5135	O	ALA	B	294	-5.383	-13.509	26.864	1.00	15.46	B
ATOM	5136	N	ASN	B	295	-6.132	-11.486	27.461	1.00	15.97	B
ATOM	5137	CA	ASN	B	295	-7.515	-11.907	27.367	1.00	17.95	B
ATOM	5138	CB	ASN	B	295	-8.052	-12.461	28.700	1.00	23.39	B
ATOM	5139	CG	ASN	B	295	-8.003	-11.480	29.817	1.00	25.82	B
ATOM	5140	OD1	ASN	B	295	-8.523	-10.373	29.718	1.00	31.67	B
ATOM	5141	ND2	ASN	B	295	-7.393	-11.888	30.929	1.00	32.50	B
ATOM	5142	C	ASN	B	295	-8.325	-10.718	26.865	1.00	16.88	B
ATOM	5143	O	ASN	B	295	-7.873	-9.568	26.935	1.00	17.31	B
ATOM	5144	N	ASN	B	296	-9.499	-10.996	26.302	1.00	16.35	B
ATOM	5145	CA	ASN	B	296	-10.311	-9.920	25.755	1.00	17.61	B
ATOM	5146	CB	ASN	B	296	-10.294	-9.966	24.205	1.00	16.78	B
ATOM	5147	CG	ASN	B	296	-10.835	-11.274	23.639	1.00	17.58	B
ATOM	5148	OD1	ASN	B	296	-11.629	-11.955	24.285	1.00	19.52	B
ATOM	5149	ND2	ASN	B	296	-10.438	-11.601	22.407	1.00	18.80	B
ATOM	5150	C	ASN	B	296	-11.734	-10.022	26.306	1.00	18.87	B
ATOM	5151	O	ASN	B	296	-12.049	-10.878	27.141	1.00	18.85	B
ATOM	5152	N	PRO	B	297	-12.603	-9.111	25.877	1.00	22.70	B
ATOM	5153	CD	PRO	B	297	-12.351	-7.873	25.120	1.00	23.09	B
ATOM	5154	CA	PRO	B	297	-13.975	-9.157	26.373	1.00	25.09	B
ATOM	5155	CB	PRO	B	297	-14.586	-7.858	25.842	1.00	25.02	B
ATOM	5156	CG	PRO	B	297	-13.432	-6.952	25.666	1.00	23.49	B
ATOM	5157	C	PRO	B	297	-14.773	-10.376	25.925	1.00	26.91	B
ATOM	5158	O	PRO	B	297	-15.828	-10.638	26.490	1.00	29.58	B
ATOM	5159	N	GLU	B	298	-14.317	-11.085	24.893	1.00	28.28	B
ATOM	5160	CA	GLU	B	298	-15.033	-12.275	24.425	1.00	29.32	B
ATOM	5161	CB	GLU	B	298	-14.805	-12.487	22.919	1.00	33.72	B
ATOM	5162	CG	GLU	B	298	-15.968	-12.033	22.025	1.00	38.43	B
ATOM	5163	CD	GLU	B	298	-16.282	-10.547	22.144	1.00	42.52	B
ATOM	5164	OE1	GLU	B	298	-15.362	-9.730	21.889	1.00	43.73	B
ATOM	5165	OE2	GLU	B	298	-17.449	-10.200	22.490	1.00	43.97	B

Figure 1 (continued 52)

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ATOM	5166	C	GLU	B	298	-14.606	-13.524	25.205	1.00	28.60	B
ATOM	5167	O	GLU	B	298	-14.936	-14.643	24.817	1.00	27.81	B
ATOM	5168	N	GLN	B	299	-13.870	-13.325	26.301	1.00	27.28	B
ATOM	5169	CA	GLN	B	299	-13.431	-14.434	27.148	1.00	27.04	B
ATOM	5170	CB	GLN	B	299	-14.615	-15.356	27.468	1.00	30.88	B
ATOM	5171	CG	GLN	B	299	-15.432	-15.000	28.711	1.00	37.59	B
ATOM	5172	OE1	GLN	B	299	-15.844	-13.553	28.768	1.00	40.60	B
ATOM	5173	OE2	GLN	B	299	-15.062	-12.682	29.185	1.00	42.63	B
ATOM	5174	NE2	GLN	B	299	-17.080	-13.273	28.344	1.00	42.73	B
ATOM	5175	C	GLN	B	299	-12.326	-15.273	26.516	1.00	22.97	B
ATOM	5176	O	GLN	B	299	-12.014	-16.375	26.995	1.00	21.99	B
ATOM	5177	N	GLU	B	300	-11.762	-14.769	25.428	1.00	19.48	B
ATOM	5178	CA	GLU	B	300	-10.680	-15.479	24.756	1.00	15.67	B
ATOM	5179	CB	GLU	B	300	-10.583	-15.026	23.291	1.00	15.71	B
ATOM	5180	CG	GLU	B	300	-11.879	-15.412	22.546	1.00	16.99	B
ATOM	5181	CD	GLU	B	300	-11.936	-14.867	21.148	1.00	17.62	B
ATOM	5182	OE1	GLU	B	300	-11.425	-13.753	20.908	1.00	19.18	B
ATOM	5183	OE2	GLU	B	300	-12.507	-15.566	20.289	1.00	18.81	B
ATOM	5184	C	GLU	B	300	-9.395	-15.245	25.501	1.00	17.24	B
ATOM	5185	O	GLU	B	300	-9.223	-14.200	26.160	1.00	15.99	B
ATOM	5186	N	GLU	B	301	-8.487	-16.212	25.407	1.00	15.46	B
ATOM	5187	CA	GLU	B	301	-7.239	-16.084	26.143	1.00	16.90	B
ATOM	5188	CB	GLU	B	301	-7.305	-16.893	27.436	1.00	21.09	B
ATOM	5189	CG	GLU	B	301	-8.146	-16.367	28.543	1.00	30.92	B
ATOM	5190	CD	GLU	B	301	-7.962	-17.237	29.766	1.00	35.02	B
ATOM	5191	OE1	GLU	B	301	-6.789	-17.389	30.212	1.00	38.01	B
ATOM	5192	OE2	GLU	B	301	-8.979	-17.773	30.255	1.00	38.32	B
ATOM	5193	C	GLU	B	301	-6.073	-16.632	25.401	1.00	15.82	B
ATOM	5194	O	GLU	B	301	-6.198	-17.658	24.748	1.00	15.36	B
ATOM	5195	N	ALA	B	302	-4.931	-15.953	25.537	1.00	14.54	B
ATOM	5196	CA	ALA	B	302	-3.688	-16.427	24.943	1.00	14.01	B
ATOM	5197	CB	ALA	B	302	-3.195	-15.479	23.876	1.00	15.13	B
ATOM	5198	C	ALA	B	302	-2.644	-16.540	26.060	1.00	14.66	B
ATOM	5199	O	ALA	B	302	-2.640	-15.741	27.006	1.00	16.02	B
ATOM	5200	N	GLU	B	303	-1.782	-17.553	25.969	1.00	13.72	B
ATOM	5201	CA	GLU	B	303	-0.691	-17.712	26.953	1.00	13.49	B
ATOM	5202	CB	GLU	B	303	-1.021	-18.772	28.011	1.00	14.66	B
ATOM	5203	CG	GLU	B	303	0.164	-19.059	28.960	1.00	18.75	B
ATOM	5204	CD	GLU	B	303	-0.155	-20.148	29.970	1.00	23.21	B
ATOM	5205	OE1	GLU	B	303	-0.967	-19.881	30.873	1.00	26.03	B
ATOM	5206	OE2	GLU	B	303	0.387	-21.261	29.853	1.00	23.17	B
ATOM	5207	C	GLU	B	303	0.559	-18.156	26.209	1.00	12.96	B
ATOM	5208	O	GLU	B	303	0.502	-19.062	25.366	1.00	12.70	B
ATOM	5209	N	GLU	B	304	1.667	-17.486	26.485	1.00	11.86	B
ATOM	5210	CA	GLU	B	304	2.955	-17.833	25.880	1.00	12.51	B
ATOM	5211	CB	GLU	B	304	3.474	-16.692	24.994	1.00	12.92	B
ATOM	5212	CG	GLU	B	304	2.613	-16.412	23.768	1.00	13.88	B
ATOM	5213	CD	GLU	B	304	2.846	-17.416	22.654	1.00	16.15	B
ATOM	5214	OE1	GLU	B	304	3.836	-18.173	22.717	1.00	14.86	B
ATOM	5215	OE2	GLU	B	304	2.029	-17.448	21.702	1.00	16.52	B
ATOM	5216	C	GLU	B	304	3.958	-18.009	27.014	1.00	12.92	B
ATOM	5217	O	GLU	B	304	4.033	-17.156	27.894	1.00	13.66	B
ATOM	5218	N	ILE	B	305	4.718	-19.108	27.010	1.00	12.77	B
ATOM	5219	CA	ILE	B	305	5.738	-19.283	28.037	1.00	11.99	B
ATOM	5220	CB	ILE	B	305	5.549	-20.605	28.791	1.00	13.43	B
ATOM	5221	CG2	ILE	B	305	6.730	-20.801	29.771	1.00	14.23	B
ATOM	5222	CG1	ILE	B	305	4.211	-20.536	29.555	1.00	15.50	B
ATOM	5223	CD1	ILE	B	305	3.773	-21.908	30.095	1.00	21.38	B
ATOM	5224	O	ILE	B	305	7.074	-19.263	27.309	1.00	13.39	B
ATOM	5225	C	ILE	B	305	7.206	-19.891	26.239	1.00	14.67	B
ATOM	5226	N	LEU	B	306	8.033	-18.501	27.838	1.00	12.78	B
ATOM	5227	CA	LEU	B	306	9.363	-18.388	27.201	1.00	13.06	B
ATOM	5228	CB	LEU	B	306	9.567	-16.973	26.621	1.00	16.49	B
ATOM	5229	CG	LEU	B	306	8.629	-16.459	25.530	1.00	19.31	B
ATOM	5230	CD1	LEU	B	306	8.803	-14.943	25.356	1.00	22.78	B
ATOM	5231	CD2	LEU	B	306	8.922	-17.216	24.223	1.00	21.99	B
ATOM	5232	C	LEU	B	306	10.473	-18.598	28.221	1.00	13.14	B
ATOM	5233	O	LEU	B	306	10.347	-18.191	29.368	1.00	13.66	B
ATOM	5234	N	ASP	B	307	11.579	-19.197	27.784	1.00	14.05	B
ATOM	5235	CA	ASP	B	307	12.724	-19.322	28.668	1.00	14.97	B
ATOM	5236	CB	ASP	B	307	13.664	-20.441	28.216	1.00	17.59	B
ATOM	5237	CG	ASP	B	307	13.064	-21.815	28.375	1.00	21.45	B
ATOM	5238	OD1	ASP	B	307	12.257	-22.018	29.283	1.00	21.70	B
ATOM	5239	OD2	ASP	B	307	13.415	-22.718	27.587	1.00	29.43	B
ATOM	5240	C	ASP	B	307	13.472	-17.998	28.538	1.00	16.22	B
ATOM	5241	O	ASP	B	307	13.683	-17.502	27.407	1.00	17.41	B
ATOM	5242	N	VAL	B	308	13.856	-17.419	29.672	1.00	15.42	B
ATOM	5243	CA	VAL	B	308	14.622	-16.170	29.691	1.00	16.59	B
ATOM	5244	CB	VAL	B	308	13.719	-14.932	29.974	1.00	16.08	B
ATOM	5245	CG1	VAL	B	308	12.596	-14.869	28.938	1.00	14.76	B
ATOM	5246	CG2	VAL	B	308	13.156	-14.972	31.412	1.00	15.53	B
ATOM	5247	C	VAL	B	308	15.661	-16.311	30.800	1.00	18.09	B
ATOM	5248	O	VAL	B	308	15.705	-17.332	31.479	1.00	18.24	B
ATOM	5249	N	THR	B	309	16.540	-15.320	30.928	1.00	17.26	B
ATOM	5250	CA	THR	B	309	17.514	-15.322	32.010	1.00	19.28	B
ATOM	5251	CB	THR	B	309	18.901	-14.815	31.545	1.00	19.61	B
ATOM	5252	CG1	THR	B	309	19.416	-15.679	30.540	1.00	21.13	B
ATOM	5253	CG2	THR	B	309	19.879	-14.794	32.712	1.00	23.93	B
ATOM	5254	C	THR	B	309	16.944	-14.334	33.032	1.00	18.30	B
ATOM	5255	O	THR	B	309	16.798	-13.147	32.747	1.00	20.11	B
ATOM	5256	N	TYR	B	310	16.577	-14.826	34.215	1.00	18.66	B
ATOM	5257	CA	TYR	B	310	16.037	-13.957	35.261	1.00	16.85	B
ATOM	5258	CB	TYR	B	310	14.537	-13.655	35.065	1.00	17.90	B
ATOM	5259	CG	TYR	B	310	13.993	-12.756	36.152	1.00	18.11	B
ATOM	5260	CD1	TYR	B	310	14.389	-11.420	36.234	1.00	19.98	B
ATOM	5261	CD2	TYR	B	310	13.958	-10.596	37.265	1.00	21.65	B
ATOM	5262	CE1	TYR	B	310	13.135	-13.241	37.142	1.00	18.77	B
ATOM	5263	CE2	TYR	B	310	12.694	-12.428	38.168	1.00	19.14	B
ATOM	5264	CZ	TYR	B	310	13.100	-11.111	38.239	1.00	22.59	B
ATOM	5265	OH	TYR	B	310	12.642	-10.325	39.276	1.00	23.29	B

Figure 1 (continued 53)

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ATOM	5266	C	TYR	B	310	16.202	-14.605	36.635	1.00	20.33	B
ATOM	5267	O	TYR	B	310	15.861	-15.775	36.802	1.00	18.99	B
ATOM	5268	N	SER	B	311	16.711	-13.831	37.604	1.00	21.68	B
ATOM	5269	CA	SER	B	311	16.890	-14.340	38.973	1.00	25.75	B
ATOM	5270	CB	SER	B	311	18.376	-14.490	39.291	1.00	27.17	B
ATOM	5271	OG	SER	B	311	18.819	-15.761	38.877	1.00	32.61	B
ATOM	5272	C	SER	B	311	16.229	-13.539	40.094	1.00	27.05	B
ATOM	5273	O	SER	B	311	16.370	-13.876	41.264	1.00	31.83	B
ATOM	5274	N	GLY	B	312	15.500	-12.481	39.778	1.00	28.46	B
ATOM	5275	CA	GLY	B	312	14.864	-11.724	40.848	1.00	28.43	B
ATOM	5276	C	GLY	B	312	13.588	-12.299	41.478	1.00	27.94	B
ATOM	5277	O	GLY	B	312	13.187	-13.451	41.239	1.00	26.97	B
ATOM	5278	N	ALA	B	313	12.957	-11.478	42.310	1.00	26.88	B
ATOM	5279	CA	ALA	B	313	11.711	-11.848	42.966	1.00	24.05	B
ATOM	5280	CB	ALA	B	313	11.312	-10.763	43.966	1.00	24.56	B
ATOM	5281	C	ALA	B	313	10.665	-11.932	41.853	1.00	22.56	B
ATOM	5282	O	ALA	B	313	10.806	-11.298	40.799	1.00	20.08	B
ATOM	5283	N	GLU	B	314	9.618	-12.725	42.066	1.00	19.40	B
ATOM	5284	CA	GLU	B	314	8.586	-12.840	41.042	1.00	18.07	B
ATOM	5285	CB	GLU	B	314	7.647	-14.039	41.323	1.00	16.92	B
ATOM	5286	CG	GLU	B	314	8.410	-15.354	41.405	1.00	16.41	B
ATOM	5287	CD	GLU	B	314	7.525	-16.589	41.365	1.00	14.40	B
ATOM	5288	OE1	GLU	B	314	6.317	-16.485	41.643	1.00	15.57	B
ATOM	5289	OE2	GLU	B	314	8.058	-17.668	41.064	1.00	17.05	B
ATOM	5290	C	GLU	B	314	7.772	-11.565	41.032	1.00	17.69	B
ATOM	5291	O	GLU	B	314	7.685	-10.870	42.033	1.00	18.99	B
ATOM	5292	N	MET	B	315	7.209	-11.226	39.878	1.00	18.30	B
ATOM	5293	CA	MET	B	315	6.352	-10.044	39.793	1.00	16.99	B
ATOM	5294	CB	MET	B	315	7.156	-8.741	39.754	1.00	19.43	B
ATOM	5295	CG	MET	B	315	8.052	-8.587	38.571	1.00	18.90	B
ATOM	5296	SD	MET	B	315	8.654	-6.862	38.490	1.00	23.78	B
ATOM	5297	CE	MET	B	315	7.247	-6.033	37.765	1.00	21.20	B
ATOM	5298	C	MET	B	315	5.509	-10.144	38.542	1.00	18.24	B
ATOM	5299	O	MET	B	315	5.833	-10.890	37.618	1.00	16.64	B
ATOM	5300	N	GLU	B	316	4.404	-9.423	38.554	1.00	17.91	B
ATOM	5301	CA	GLU	B	316	3.499	-9.387	37.442	1.00	19.14	B
ATOM	5302	CB	GLU	B	316	2.153	-9.964	37.876	1.00	22.45	B
ATOM	5303	CG	GLU	B	316	1.183	-10.293	36.755	1.00	30.42	B
ATOM	5304	CD	GLU	B	316	-0.058	-11.022	37.282	1.00	33.19	B
ATOM	5305	OE1	GLU	B	316	-0.126	-12.269	37.189	1.00	36.29	B
ATOM	5306	OE2	GLU	B	316	-0.957	-10.337	37.807	1.00	35.89	B
ATOM	5307	C	GLU	B	316	3.174	-7.316	37.058	1.00	18.61	B
ATOM	5308	O	GLU	B	316	3.442	-7.029	37.917	1.00	19.48	B
ATOM	5309	N	ILE	B	317	3.202	-7.651	35.770	1.00	17.17	B
ATOM	5310	CA	ILE	B	317	3.090	-6.281	35.317	1.00	14.40	B
ATOM	5311	CB	ILE	B	317	4.500	-5.648	35.163	1.00	14.99	B
ATOM	5312	CG2	ILE	B	317	5.382	-6.449	34.166	1.00	15.39	B
ATOM	5313	CG1	ILE	B	317	4.373	-4.195	34.724	1.00	16.07	B
ATOM	5314	CD1	ILE	B	317	5.731	-3.450	34.830	1.00	16.39	B
ATOM	5315	C	ILE	B	317	2.319	-6.249	34.003	1.00	15.31	B
ATOM	5316	O	ILE	B	317	2.484	-7.144	33.166	1.00	15.36	B
ATOM	5317	N	GLY	B	318	1.489	-5.225	33.826	1.00	15.37	B
ATOM	5318	CA	GLY	B	318	0.701	-5.121	32.611	1.00	13.91	B
ATOM	5319	C	GLY	B	318	1.261	-4.061	31.670	1.00	15.48	B
ATOM	5320	O	GLY	B	318	1.888	-3.115	32.135	1.00	14.18	B
ATOM	5321	N	PHE	B	319	1.072	-4.255	30.363	1.00	15.89	B
ATOM	5322	CA	PHE	B	319	1.513	-3.311	29.331	1.00	16.03	B
ATOM	5323	CB	PHE	B	319	2.897	-3.692	28.777	1.00	17.13	B
ATOM	5324	CG	PHE	B	319	4.022	-3.383	29.686	1.00	18.79	B
ATOM	5325	CD1	PHE	B	319	4.434	-2.073	29.877	1.00	21.89	B
ATOM	5326	CD2	PHE	B	319	4.673	-4.401	30.368	1.00	21.55	B
ATOM	5327	CE1	PHE	B	319	5.481	-1.786	30.740	1.00	22.47	B
ATOM	5328	CE2	PHE	B	319	5.716	-4.122	31.236	1.00	21.80	B
ATOM	5329	CZ	PHE	B	319	6.121	-2.820	31.423	1.00	23.74	B
ATOM	5330	C	PHE	B	319	0.602	-3.282	28.129	1.00	16.79	B
ATOM	5331	O	PHE	B	319	-0.122	-4.243	27.846	1.00	16.37	B
ATOM	5332	N	ASN	B	320	0.635	-2.143	27.431	1.00	16.27	B
ATOM	5333	CA	ASN	B	320	-0.051	-1.983	26.158	1.00	16.46	B
ATOM	5334	CB	ASN	B	320	-0.055	-0.504	25.796	1.00	18.69	B
ATOM	5335	CG	ASN	B	320	-0.561	-0.259	24.407	1.00	18.32	B
ATOM	5336	OD1	ASN	B	320	-0.226	-0.997	23.481	1.00	18.44	B
ATOM	5337	ND2	ASN	B	320	-1.362	0.791	24.242	1.00	18.81	B
ATOM	5338	C	ASN	B	320	0.927	-2.745	25.249	1.00	17.08	B
ATOM	5339	O	ASN	B	320	2.093	-2.350	25.102	1.00	16.27	B
ATOM	5340	N	VAL	B	321	0.478	-3.843	24.645	1.00	15.94	B
ATOM	5341	CA	VAL	B	321	1.379	-4.662	23.845	1.00	16.35	B
ATOM	5342	CB	VAL	B	321	0.703	-6.027	23.464	1.00	16.49	B
ATOM	5343	CG1	VAL	B	321	-0.409	-5.817	22.450	1.00	17.69	B
ATOM	5344	CG2	VAL	B	321	1.743	-7.004	22.956	1.00	14.64	B
ATOM	5345	C	VAL	B	321	1.891	-3.939	22.610	1.00	17.10	B
ATOM	5346	O	VAL	B	321	2.977	-4.245	22.119	1.00	15.35	B
ATOM	5347	N	SER	B	322	1.146	-2.961	22.109	1.00	16.12	B
ATOM	5348	CA	SER	B	322	1.657	-3.257	20.925	1.00	17.12	B
ATOM	5349	CB	SER	B	322	0.587	-1.352	20.311	1.00	18.39	B
ATOM	5350	CG	SER	B	322	-0.513	-2.129	19.863	1.00	22.65	B
ATOM	5351	C	SER	B	322	2.899	-1.436	21.276	1.00	15.98	B
ATOM	5352	O	SER	B	322	3.837	-1.353	20.468	1.00	15.16	B
ATOM	5353	N	TYR	B	323	2.932	-0.853	22.482	1.00	14.24	B
ATOM	5354	CA	TYR	B	323	4.110	-0.088	22.908	1.00	15.80	B
ATOM	5355	CB	TYR	B	323	3.878	0.590	24.259	1.00	15.47	B
ATOM	5356	CG	TYR	B	323	2.813	1.668	24.294	1.00	16.35	B
ATOM	5357	CD1	TYR	B	323	2.397	2.314	23.127	1.00	19.59	B
ATOM	5358	CE1	TYR	B	323	1.456	3.374	23.170	1.00	20.04	B
ATOM	5359	CD2	TYR	B	323	2.284	2.093	25.509	1.00	18.22	B
ATOM	5360	CE2	TYR	B	323	1.354	3.166	25.567	1.00	19.75	B
ATOM	5361	CZ	TYR	B	323	0.957	3.790	24.399	1.00	21.19	B
ATOM	5362	OH	TYR	B	323	0.112	4.886	24.453	1.00	23.64	B
ATOM	5363	C	TYR	B	323	5.327	-1.018	23.041	1.00	15.80	B
ATOM	5364	O	TYR	B	323	6.468	-0.646	22.726	1.00	15.87	B
ATOM	5365	N	VAL	B	324	5.101	-2.226	23.563	1.00	14.85	B

Figure 1 (continued 54)

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ATOM	5366	CA	VAL	B	324	6.193	-3.182	23.687	1.00	14.69	B
ATOM	5367	CB	VAL	B	324	5.776	-4.387	24.550	1.00	14.90	B
ATOM	5368	CG1	VAL	B	324	6.913	-5.422	24.610	1.00	16.80	B
ATOM	5369	CG2	VAL	B	324	5.440	-3.896	25.952	1.00	16.82	B
ATOM	5370	C	VAL	B	324	6.674	-3.670	22.301	1.00	13.75	B
ATOM	5371	O	VAL	B	324	7.885	-3.761	22.039	1.00	14.44	B
ATOM	5372	N	LEU	B	325	5.737	-3.984	21.410	1.00	14.44	B
ATOM	5373	CA	LEU	B	325	6.105	-4.424	20.085	1.00	13.52	B
ATOM	5374	CB	LEU	B	325	4.852	-4.870	19.317	1.00	14.38	B
ATOM	5375	CG	LEU	B	325	4.339	-6.244	19.774	1.00	14.30	B
ATOM	5376	CD1	LEU	B	325	2.953	-6.506	19.170	1.00	15.19	B
ATOM	5377	CD2	LEU	B	325	5.338	-7.346	19.363	1.00	14.63	B
ATOM	5378	C	LEU	B	325	6.848	-3.319	19.334	1.00	14.06	B
ATOM	5379	O	LEU	B	325	7.801	-3.603	18.606	1.00	15.63	B
ATOM	5380	N	ASP	B	326	6.420	-2.074	19.503	1.00	14.14	B
ATOM	5381	CA	ASP	B	326	7.113	-0.960	18.843	1.00	14.45	B
ATOM	5382	CB	ASP	B	326	6.505	0.385	19.217	1.00	15.89	B
ATOM	5383	CG	ASP	B	326	5.168	0.634	18.556	1.00	16.26	B
ATOM	5384	OD1	ASP	B	326	4.803	-0.036	17.556	1.00	17.26	B
ATOM	5385	OD2	ASP	B	326	4.471	1.551	19.018	1.00	18.69	B
ATOM	5386	C	ASP	B	326	8.588	-0.952	19.255	1.00	14.86	B
ATOM	5387	O	ASP	B	326	9.454	-0.768	18.416	1.00	15.93	B
ATOM	5388	N	VAL	B	327	8.871	-1.163	20.542	1.00	15.32	B
ATOM	5389	CA	VAL	B	327	10.246	-1.175	20.989	1.00	15.55	B
ATOM	5390	CB	VAL	B	327	10.301	-1.226	22.534	1.00	16.32	B
ATOM	5391	CG1	VAL	B	327	11.715	-1.474	22.996	1.00	15.81	B
ATOM	5392	CG2	VAL	B	327	9.783	0.086	23.085	1.00	15.65	B
ATOM	5393	C	VAL	B	327	11.039	-2.352	20.422	1.00	16.20	B
ATOM	5394	O	VAL	B	327	12.179	-2.184	19.974	1.00	15.94	B
ATOM	5395	N	LEU	B	328	10.437	-3.547	20.435	1.00	14.84	B
ATOM	5396	CA	LEU	B	328	11.150	-4.726	19.961	1.00	15.54	B
ATOM	5397	CB	LEU	B	328	10.347	-5.985	20.295	1.00	14.62	B
ATOM	5398	CG	LEU	B	328	10.130	-6.193	21.808	1.00	15.10	B
ATOM	5399	CD1	LEU	B	328	9.295	-7.460	22.024	1.00	14.68	B
ATOM	5400	CD2	LEU	B	328	11.503	-6.337	22.487	1.00	16.58	B
ATOM	5401	C	LEU	B	328	11.416	-4.600	18.480	1.00	16.34	B
ATOM	5402	O	LEU	B	328	12.455	-5.042	17.998	1.00	17.56	B
ATOM	5403	N	ASN	B	329	10.491	-3.970	17.758	1.00	17.06	B
ATOM	5404	CA	ASN	B	329	10.680	-3.755	16.332	1.00	20.23	B
ATOM	5405	CB	ASN	B	329	9.371	-3.285	15.675	1.00	20.68	B
ATOM	5406	CG	ASN	B	329	8.414	-4.440	15.381	1.00	25.15	B
ATOM	5407	OD1	ASN	B	329	7.193	-4.308	15.536	1.00	29.33	B
ATOM	5408	ND2	ASN	B	329	8.961	-5.571	14.932	1.00	25.44	B
ATOM	5409	C	ASN	B	329	11.790	-2.743	16.076	1.00	20.26	B
ATOM	5410	O	ASN	B	329	12.504	-2.875	15.074	1.00	21.57	B
ATOM	5411	N	ALA	B	330	11.958	-1.754	16.963	1.00	20.54	B
ATOM	5412	CA	ALA	B	330	13.007	-0.741	16.795	1.00	20.36	B
ATOM	5413	CB	ALA	B	330	12.703	0.488	17.630	1.00	19.00	B
ATOM	5414	C	ALA	B	330	14.392	-1.275	17.151	1.00	22.18	B
ATOM	5415	O	ALA	B	330	15.410	-0.786	16.652	1.00	22.02	B
ATOM	5416	N	LEU	B	331	14.425	-2.269	18.031	1.00	22.79	B
ATOM	5417	CA	LEU	B	331	15.675	-2.900	18.445	1.00	26.40	B
ATOM	5418	CB	LEU	B	331	15.542	-3.459	19.876	1.00	24.34	B
ATOM	5419	CG	LEU	B	331	15.521	-2.496	21.077	1.00	23.11	B
ATOM	5420	CD1	LEU	B	331	15.059	-3.251	22.320	1.00	23.07	B
ATOM	5421	CD2	LEU	B	331	16.904	-1.904	21.324	1.00	22.88	B
ATOM	5422	C	LEU	B	331	15.953	-4.042	17.466	1.00	29.87	B
ATOM	5423	O	LEU	B	331	15.346	-5.118	17.543	1.00	32.92	B
ATOM	5424	N	LYS	B	332	16.871	-3.831	16.540	1.00	32.35	B
ATOM	5425	CA	LYS	B	332	17.157	-4.892	15.576	1.00	34.77	B
ATOM	5426	CB	LYS	B	332	17.447	-4.281	14.205	1.00	37.40	B
ATOM	5427	CG	LYS	B	332	18.504	-3.195	14.249	1.00	41.60	B
ATOM	5428	CD	LYS	B	332	18.968	-2.812	12.865	1.00	44.04	B
ATOM	5429	CE	LYS	B	332	20.404	-2.327	12.925	1.00	46.03	B
ATOM	5430	NZ	LYS	B	332	21.304	-3.408	13.449	1.00	46.84	B
ATOM	5431	C	LYS	B	332	18.364	-5.647	16.110	1.00	34.26	B
ATOM	5432	O	LYS	B	332	19.478	-5.520	15.583	1.00	36.38	B
ATOM	5433	N	CYS	B	333	18.139	-6.428	17.167	1.00	31.45	B
ATOM	5434	CA	CYS	B	333	19.227	-7.147	17.809	1.00	38.74	B
ATOM	5435	CB	CYS	B	333	19.682	-6.364	19.040	1.00	26.65	B
ATOM	5436	SG	CYS	B	333	18.382	-6.128	20.301	1.00	24.29	B
ATOM	5437	C	CYS	B	333	18.900	-8.582	18.201	1.00	27.77	B
ATOM	5438	O	CYS	B	333	17.771	-9.039	18.057	1.00	27.74	B
ATOM	5439	N	GLU	B	334	19.891	-9.292	18.722	1.00	24.94	B
ATOM	5440	CA	GLU	B	334	19.651	-10.671	19.072	1.00	25.13	B
ATOM	5441	CB	GLU	B	334	20.940	-11.490	19.059	1.00	28.75	B
ATOM	5442	CG	GLU	B	334	20.639	-12.973	18.832	1.00	33.58	B
ATOM	5443	CD	GLU	B	334	21.798	-13.903	19.171	1.00	37.85	B
ATOM	5444	OE1	GLU	B	334	22.835	-13.880	18.469	1.00	38.76	B
ATOM	5445	OE2	GLU	B	334	21.656	-14.670	20.151	1.00	39.90	B
ATOM	5446	C	GLU	B	334	18.977	-10.831	20.420	1.00	22.72	B
ATOM	5447	O	GLU	B	334	18.060	-11.628	20.559	1.00	22.05	B
ATOM	5448	N	ASN	B	335	19.449	-10.089	21.410	1.00	21.54	B
ATOM	5449	CA	ASN	B	335	18.873	-10.202	22.751	1.00	21.37	B
ATOM	5450	CB	ASN	B	335	19.841	-10.945	23.673	1.00	22.21	B
ATOM	5451	CG	ASN	B	335	20.230	-12.327	23.127	1.00	23.10	B
ATOM	5452	OD1	ASN	B	335	21.320	-12.515	22.569	1.00	27.23	B
ATOM	5453	ND2	ASN	B	335	19.349	-13.283	23.283	1.00	20.66	B
ATOM	5454	C	ASN	B	335	18.540	-8.849	23.347	1.00	21.05	B
ATOM	5455	O	ASN	B	335	19.193	-7.848	23.057	1.00	19.95	B
ATOM	5456	N	VAL	B	336	17.499	-8.824	24.174	1.00	18.30	B
ATOM	5457	CA	VAL	B	336	17.074	-7.600	24.817	1.00	18.62	B
ATOM	5458	CB	VAL	B	336	15.629	-7.224	24.418	1.00	19.11	B
ATOM	5459	CG1	VAL	B	336	15.564	-6.941	22.908	1.00	19.33	B
ATOM	5460	CG2	VAL	B	336	14.681	-8.367	24.762	1.00	23.69	B
ATOM	5461	C	VAL	B	336	17.118	-7.770	26.331	1.00	19.78	B
ATOM	5462	O	VAL	B	336	17.054	-8.896	26.846	1.00	20.30	B
ATOM	5463	N	ARG	B	337	17.243	-6.644	27.022	1.00	18.96	B
ATOM	5464	CA	ARG	B	337	17.259	-6.617	28.482	1.00	19.16	B
ATOM	5465	CB	ARG	B	337	18.589	-6.071	29.016	1.00	20.68	B

Figure 1 (continued 55)

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ATOM	5466	CG	ARG	B	337	18.600	-5.938	30.554	1.00	23.91	B
ATOM	5467	CD	ARG	B	337	19.995	-5.583	31.102	1.00	23.98	B
ATOM	5468	NE	ARG	B	337	21.011	-6.545	30.668	1.00	27.10	B
ATOM	5469	CZ	ARG	B	337	21.895	-6.313	29.704	1.00	26.89	B
ATOM	5470	NH1	ARG	B	337	21.898	-5.149	29.068	1.00	28.48	B
ATOM	5471	NH2	ARG	B	337	22.773	-7.244	29.371	1.00	28.51	B
ATOM	5472	C	ARG	B	337	16.134	-5.715	28.938	1.00	19.09	B
ATOM	5473	O	ARG	B	337	15.996	-4.586	28.465	1.00	18.29	B
ATOM	5474	N	MET	B	338	15.293	-6.223	29.835	1.00	18.31	B
ATOM	5475	CA	MET	B	338	14.197	-5.456	30.392	1.00	19.62	B
ATOM	5476	CB	MET	B	338	12.884	-6.241	30.331	1.00	20.28	B
ATOM	5477	CG	MET	B	338	12.410	-6.552	28.924	1.00	23.02	B
ATOM	5478	SD	MET	B	338	10.698	-7.188	28.918	1.00	30.58	B
ATOM	5479	CE	MET	B	338	10.105	-6.371	30.539	1.00	23.41	B
ATOM	5480	C	MET	B	338	14.585	-5.245	31.843	1.00	19.01	B
ATOM	5481	O	MET	B	338	14.968	-6.203	32.527	1.00	19.47	B
ATOM	5482	CO	MET	B	339	14.491	-4.008	32.302	1.00	20.01	B
ATOM	5483	CA	MET	B	339	14.840	-3.658	33.682	1.00	19.93	B
ATOM	5484	CB	MET	B	339	15.951	-2.600	33.651	1.00	23.82	B
ATOM	5485	CG	MET	B	339	17.044	-3.049	32.682	1.00	28.37	B
ATOM	5486	SD	MET	B	339	18.055	-1.714	32.046	1.00	39.00	B
ATOM	5487	CE	MET	B	339	19.307	-1.887	33.240	1.00	33.07	B
ATOM	5488	C	MET	B	339	19.570	-3.191	34.385	1.00	18.83	B
ATOM	5489	O	MET	B	339	12.958	-2.204	34.009	1.00	16.91	B
ATOM	5490	N	LEU	B	340	13.174	-3.940	35.420	1.00	18.32	B
ATOM	5491	CA	LEU	B	340	11.927	-3.673	36.114	1.00	20.68	B
ATOM	5492	CB	LEU	B	340	11.036	-4.916	36.055	1.00	23.79	B
ATOM	5493	CG	LEU	B	340	10.657	-5.377	34.649	1.00	25.40	B
ATOM	5494	CD1	LEU	B	340	11.509	-6.576	34.276	1.00	29.66	B
ATOM	5495	CD2	LEU	B	340	9.190	-5.735	34.630	1.00	28.50	B
ATOM	5496	C	LEU	B	340	12.104	-3.309	37.555	1.00	19.92	B
ATOM	5497	O	LEU	B	340	13.150	-3.553	38.135	1.00	21.79	B
ATOM	5498	N	THR	B	341	11.055	-2.720	38.116	1.00	23.10	B
ATOM	5499	CA	THR	B	341	11.045	-2.310	39.509	1.00	25.27	B
ATOM	5500	CB	THR	B	341	10.910	-0.789	39.596	1.00	26.79	B
ATOM	5501	CG1	THR	B	341	12.026	-0.190	38.911	1.00	28.09	B
ATOM	5502	CG2	THR	B	341	10.904	-0.337	41.053	1.00	26.69	B
ATOM	5503	C	THR	B	341	9.863	-3.015	40.164	1.00	28.85	B
ATOM	5504	O	THR	B	341	10.041	-3.872	41.028	1.00	28.86	B
ATOM	5505	N	ASP	B	342	8.653	-2.670	39.735	1.00	25.54	B
ATOM	5506	CA	ASP	B	342	7.466	-3.300	40.266	1.00	25.04	B
ATOM	5507	CB	ASP	B	342	7.138	-2.742	41.651	1.00	25.70	B
ATOM	5508	CG	ASP	B	342	6.999	-1.236	41.650	1.00	27.01	B
ATOM	5509	OD1	ASP	B	342	6.409	-0.692	40.701	1.00	23.85	B
ATOM	5510	OD2	ASP	B	342	7.474	-0.587	42.615	1.00	29.24	B
ATOM	5511	C	ASP	B	342	6.309	-3.091	39.312	1.00	26.03	B
ATOM	5512	O	ASP	B	342	6.469	-2.510	38.235	1.00	23.30	B
ATOM	5513	N	SER	B	343	5.140	-3.581	39.700	1.00	24.53	B
ATOM	5514	CA	SER	B	343	3.954	-3.490	38.866	1.00	26.73	B
ATOM	5515	CB	SER	B	343	2.814	-4.253	39.519	1.00	27.90	B
ATOM	5516	CG	SER	B	343	3.278	-5.495	39.991	1.00	33.35	B
ATOM	5517	C	SER	B	343	3.445	-2.107	38.522	1.00	25.46	B
ATOM	5518	O	SER	B	343	2.683	-1.947	37.568	1.00	27.08	B
ATOM	5519	N	VAL	B	344	3.837	-1.100	39.291	1.00	25.08	B
ATOM	5520	CA	VAL	B	344	3.324	0.227	39.030	1.00	23.51	B
ATOM	5521	CB	VAL	B	344	2.676	0.818	40.318	1.00	24.60	B
ATOM	5522	CG1	VAL	B	344	1.474	-0.026	40.725	1.00	27.19	B
ATOM	5523	CG2	VAL	B	344	3.687	0.847	41.456	1.00	24.67	B
ATOM	5524	C	VAL	B	344	4.405	1.163	38.512	1.00	23.49	B
ATOM	5525	O	VAL	B	344	4.199	2.365	38.405	1.00	23.89	B
ATOM	5526	N	SER	B	345	5.550	0.607	38.151	1.00	21.31	B
ATOM	5527	CA	SER	B	345	6.617	1.467	37.691	1.00	20.87	B
ATOM	5528	CB	SER	B	345	7.810	1.318	38.627	1.00	23.30	B
ATOM	5529	CG	SER	B	345	7.409	1.696	39.946	1.00	21.45	B
ATOM	5530	C	SER	B	345	7.012	1.166	36.260	1.00	21.79	B
ATOM	5531	O	SER	B	345	6.770	0.077	35.761	1.00	21.63	B
ATOM	5532	N	SER	B	346	7.618	2.153	35.615	1.00	21.53	B
ATOM	5533	CA	SER	B	346	8.060	2.002	34.239	1.00	21.50	B
ATOM	5534	CB	SER	B	346	8.655	3.320	33.722	1.00	21.47	B
ATOM	5535	CG	SER	B	346	9.793	3.703	34.474	1.00	26.08	B
ATOM	5536	C	SER	B	346	9.107	0.914	34.106	1.00	20.70	B
ATOM	5537	O	SER	B	346	9.755	0.521	35.078	1.00	21.55	B
ATOM	5538	N	VAL	B	347	9.255	0.411	32.890	1.00	21.06	B
ATOM	5539	CA	VAL	B	347	10.254	-0.589	32.610	1.00	19.47	B
ATOM	5540	CB	VAL	B	347	9.667	-1.886	31.960	1.00	21.64	B
ATOM	5541	CG1	VAL	B	347	9.016	-1.578	30.636	1.00	22.58	B
ATOM	5542	CG2	VAL	B	347	10.767	-2.905	31.746	1.00	22.90	B
ATOM	5543	C	VAL	B	347	11.171	0.054	31.582	1.00	19.98	B
ATOM	5544	O	VAL	B	347	10.705	0.845	30.758	1.00	19.77	B
ATOM	5545	N	GLN	B	348	12.447	-0.270	31.667	1.00	18.29	B
ATOM	5546	CA	GLN	B	348	13.421	0.211	30.694	1.00	19.12	B
ATOM	5547	CB	GLN	B	348	14.667	0.811	31.375	1.00	21.07	B
ATOM	5548	CG	GLN	B	348	15.791	1.231	30.385	1.00	24.52	B
ATOM	5549	CD	GLN	B	348	16.826	2.140	31.039	1.00	25.62	B
ATOM	5550	OE1	GLN	B	348	18.017	2.109	30.692	1.00	29.04	B
ATOM	5551	NE2	GLN	B	348	16.378	2.944	31.980	1.00	25.26	B
ATOM	5552	C	GLN	B	348	13.827	-0.987	29.863	1.00	18.81	B
ATOM	5553	O	GLN	B	348	14.128	-2.070	30.398	1.00	19.57	B
ATOM	5554	N	ILE	B	349	13.828	-0.811	28.539	1.00	16.48	B
ATOM	5555	CA	ILE	B	349	14.216	-1.893	27.640	1.00	16.69	B
ATOM	5556	CB	ILE	B	349	13.043	-2.317	26.739	1.00	15.20	B
ATOM	5557	CG2	ILE	B	349	13.450	-3.542	25.886	1.00	15.51	B
ATOM	5558	CG1	ILE	B	349	11.814	-2.594	27.628	1.00	14.39	B
ATOM	5559	CD1	ILE	B	349	10.543	-2.916	26.841	1.00	16.74	B
ATOM	5560	C	ILE	B	349	15.354	-1.434	26.757	1.00	16.84	B
ATOM	5561	O	ILE	B	349	15.342	-0.309	26.258	1.00	17.09	B
ATOM	5562	N	GLU	B	350	16.316	-2.315	26.555	1.00	18.33	B
ATOM	5563	CA	GLU	B	350	17.477	-2.012	25.717	1.00	20.07	B
ATOM	5564	CB	GLU	B	350	18.606	-1.403	26.573	1.00	22.27	B
ATOM	5565	CG	GLU	B	350	18.629	-1.904	28.009	1.00	27.54	B

Figure 1 (continued 56)

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ATOM	5566	CD	GLU	B	350	19.768	-1.317	28.861	1.00	28.87	B
ATOM	5567	OE1	GLU	B	350	19.985	-0.085	28.838	1.00	30.71	B
ATOM	5568	OE2	GLU	B	350	20.435	-2.111	29.569	1.00	32.23	B
ATOM	5569	C	GLU	B	350	18.018	-3.247	25.033	1.00	20.43	B
ATOM	5570	O	GLU	B	350	17.663	-4.385	25.373	1.00	19.39	B
ATOM	5571	N	ASP	B	351	18.864	-3.023	24.030	1.00	18.78	B
ATOM	5572	CA	ASP	B	351	19.556	-4.127	23.383	1.00	20.40	B
ATOM	5573	CB	ASP	B	351	20.393	-3.559	22.216	1.00	20.92	B
ATOM	5574	CG	ASP	B	351	21.276	-4.593	21.540	1.00	24.22	B
ATOM	5575	OD1	ASP	B	351	21.520	-5.668	22.122	1.00	23.24	B
ATOM	5576	OD2	ASP	B	351	21.747	-4.326	20.399	1.00	24.36	B
ATOM	5577	O	ASP	B	351	20.480	-4.641	24.519	1.00	20.22	B
ATOM	5578	N	ASP	B	351	21.154	-3.837	25.166	1.00	19.94	B
ATOM	5579	CA	ALA	B	352	20.513	-5.955	24.767	1.00	20.14	B
ATOM	5580	CB	ALA	B	352	21.371	-6.512	25.828	1.00	22.88	B
ATOM	5581	O	ALA	B	352	21.102	-8.023	25.989	1.00	23.61	B
ATOM	5582	CA	ALA	B	352	22.856	-6.282	25.541	1.00	25.05	B
ATOM	5583	CB	ALA	B	352	23.687	-6.298	26.459	1.00	25.32	B
ATOM	5584	N	ALA	B	353	23.187	-6.059	24.272	1.00	25.32	B
ATOM	5585	CA	ALA	B	353	24.583	-5.871	23.874	1.00	27.92	B
ATOM	5586	CB	ALA	B	353	24.888	-6.727	22.622	1.00	28.12	B
ATOM	5587	O	ALA	B	353	25.008	-4.429	23.628	1.00	29.48	B
ATOM	5588	N	ALA	B	353	26.134	-4.185	23.189	1.00	30.65	B
ATOM	5589	CA	SER	B	354	24.130	-3.471	23.895	1.00	28.82	B
ATOM	5590	CB	SER	B	354	24.491	-2.068	23.695	1.00	30.09	B
ATOM	5591	O	SER	B	354	24.439	-1.695	22.213	1.00	30.87	B
ATOM	5592	CA	SER	B	354	24.378	-0.282	22.073	1.00	30.83	B
ATOM	5593	CB	SER	B	354	23.612	-1.097	24.458	1.00	29.65	B
ATOM	5594	O	SER	B	354	22.382	-1.233	24.488	1.00	29.50	B
ATOM	5595	N	GLN	B	355	24.236	-0.096	25.064	1.00	29.47	B
ATOM	5596	CA	GLN	B	355	23.475	0.900	25.794	1.00	29.78	B
ATOM	5597	CB	GLN	B	355	24.227	1.337	27.057	1.00	33.08	B
ATOM	5598	O	GLN	B	355	24.449	0.245	28.091	1.00	37.90	B
ATOM	5599	CD	GLN	B	355	25.421	0.691	29.180	1.00	41.35	B
ATOM	5600	OE1	GLN	B	355	26.640	0.756	28.959	1.00	42.13	B
ATOM	5601	NE2	GLN	B	355	24.883	1.026	30.355	1.00	42.11	B
ATOM	5602	C	GLN	B	355	23.230	2.117	24.896	1.00	29.04	B
ATOM	5603	O	GLN	B	355	22.833	3.167	25.389	1.00	29.11	B
ATOM	5604	N	SER	B	356	23.439	1.963	23.586	1.00	28.20	B
ATOM	5605	CA	SER	B	356	23.247	3.072	22.630	1.00	28.53	B
ATOM	5606	CB	SER	B	356	23.499	2.600	21.187	1.00	29.22	B
ATOM	5607	O	SER	B	356	24.878	2.462	20.908	1.00	33.92	B
ATOM	5608	C	SER	B	356	21.839	3.659	23.699	1.00	26.91	B
ATOM	5609	N	SER	B	356	21.636	4.883	22.644	1.00	26.04	B
ATOM	5610	CA	ALA	B	357	20.849	2.782	22.801	1.00	24.78	B
ATOM	5611	CB	ALA	B	357	19.476	3.240	22.852	1.00	23.09	B
ATOM	5612	O	ALA	B	357	18.707	2.773	21.599	1.00	23.03	B
ATOM	5613	N	ALA	B	357	18.795	2.702	24.099	1.00	23.24	B
ATOM	5614	CA	ALA	B	357	19.167	1.645	24.625	1.00	25.22	B
ATOM	5615	CB	ALA	B	358	17.825	3.457	24.587	1.00	21.13	B
ATOM	5616	O	ALA	B	358	17.055	3.030	25.747	1.00	21.52	B
ATOM	5617	N	ALA	B	358	17.643	3.649	27.031	1.00	22.50	B
ATOM	5618	CA	ALA	B	358	15.585	3.402	25.566	1.00	19.54	B
ATOM	5619	CB	ALA	B	358	15.257	4.451	25.037	1.00	18.37	B
ATOM	5620	O	TYR	B	359	14.683	2.527	26.017	1.00	18.21	B
ATOM	5621	N	TYR	B	359	13.259	2.747	25.886	1.00	18.06	B
ATOM	5622	CA	TYR	B	359	12.642	1.724	24.919	1.00	17.72	B
ATOM	5623	CB	TYR	B	359	13.303	1.776	23.558	1.00	15.03	B
ATOM	5624	OD1	TYR	B	359	14.473	1.076	23.300	1.00	16.16	B
ATOM	5625	OE1	TYR	B	359	15.151	1.242	22.104	1.00	14.13	B
ATOM	5626	OD2	TYR	B	359	12.812	2.648	22.573	1.00	15.69	B
ATOM	5627	OE2	TYR	B	359	13.485	2.819	21.379	1.00	13.85	B
ATOM	5628	CZ	TYR	B	359	14.633	2.127	21.145	1.00	15.70	B
ATOM	5629	OH	TYR	B	359	15.265	2.315	19.935	1.00	16.11	B
ATOM	5630	C	TYR	B	359	12.597	2.609	27.235	1.00	19.04	B
ATOM	5631	O	TYR	B	359	12.908	1.686	27.992	1.00	19.57	B
ATOM	5632	N	VAL	B	360	11.730	3.546	27.545	1.00	17.94	B
ATOM	5633	CA	VAL	B	360	11.023	3.501	28.812	1.00	19.18	B
ATOM	5634	CB	VAL	B	360	11.276	4.794	29.641	1.00	18.75	B
ATOM	5635	CG1	VAL	B	360	10.448	4.742	30.934	1.00	20.25	B
ATOM	5636	CG2	VAL	B	360	12.753	4.923	29.937	1.00	19.41	B
ATOM	5637	O	VAL	B	360	9.562	3.381	28.501	1.00	19.10	B
ATOM	5638	N	VAL	B	360	9.008	4.188	27.753	1.00	19.90	B
ATOM	5639	CA	VAL	B	361	8.905	2.372	29.069	1.00	19.72	B
ATOM	5640	CB	VAL	B	361	7.488	2.188	28.831	1.00	18.92	B
ATOM	5641	O	VAL	B	361	7.216	0.872	28.069	1.00	18.99	B
ATOM	5642	CG1	VAL	B	361	5.743	0.769	27.716	1.00	18.31	B
ATOM	5643	CG2	VAL	B	361	8.065	0.839	26.786	1.00	17.76	B
ATOM	5644	C	VAL	B	361	6.793	2.100	30.167	1.00	19.47	B
ATOM	5645	N	VAL	B	361	7.232	1.362	31.038	1.00	16.90	B
ATOM	5646	O	MET	B	362	5.737	2.885	30.318	1.00	20.10	B
ATOM	5647	CA	MET	B	362	4.962	2.882	31.540	1.00	21.78	B
ATOM	5648	CB	MET	B	362	4.226	4.206	31.682	1.00	24.19	B
ATOM	5649	CG	MET	B	362	3.918	4.589	33.122	1.00	27.23	B
ATOM	5650	SD	MET	B	362	5.405	4.806	34.163	1.00	29.11	B
ATOM	5651	C	MET	B	362	4.575	4.880	35.731	1.00	30.05	B
ATOM	5652	OE	MET	B	362	3.949	1.731	31.471	1.00	20.28	B
ATOM	5653	N	MET	B	362	3.385	1.438	30.410	1.00	19.68	B
ATOM	5654	CA	PRO	B	363	3.698	1.069	32.599	1.00	20.71	B
ATOM	5655	CB	PRO	B	363	4.521	1.025	33.818	1.00	21.21	B
ATOM	5656	O	PRO	B	363	2.729	-0.038	32.579	1.00	20.67	B
ATOM	5657	N	PRO	B	363	3.155	-0.883	33.776	1.00	22.57	B
ATOM	5658	CA	PRO	B	363	3.665	0.160	34.754	1.00	22.37	B
ATOM	5659	CB	PRO	B	363	1.272	0.395	32.672	1.00	22.28	B
ATOM	5660	O	PRO	B	363	0.959	1.574	32.811	1.00	18.47	B
ATOM	5661	N	MET	B	364	0.368	-0.568	32.537	1.00	23.87	B
ATOM	5662	CA	MET	B	364	-1.037	-0.272	32.674	1.00	26.94	B
ATOM	5663	CB	MET	B	364	-1.780	-0.391	31.332	1.00	29.59	B
ATOM	5664	O	MET	B	364	-1.636	-1.670	30.568	1.00	31.24	B
ATOM	5665	SD	MET	B	364	-2.386	-1.510	28.872	1.00	31.43	B

Figure 1 (continued 57)

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ATOM	5666	CE	MET	B	364	-4.155	-1.253	29.308	1.00	32.24
ATOM	5667	C	MET	B	364	-1.602	-1.218	33.725	1.00	30.19
ATOM	5668	O	MET	B	364	-0.999	-2.251	34.035	1.00	29.20
ATOM	5669	N	ARG	B	365	-2.732	-0.836	34.307	1.00	32.96
ATOM	5670	CA	ARG	B	365	-3.383	-1.655	35.324	1.00	36.74
ATOM	5671	CB	ARG	B	365	-4.029	-0.756	36.394	1.00	37.59
ATOM	5672	CG	ARG	B	365	-4.785	-1.490	37.505	1.00	39.77
ATOM	5673	CD	ARG	B	365	-3.859	-2.316	38.398	1.00	40.23
ATOM	5674	NE	ARG	B	365	-4.571	-2.956	39.505	1.00	40.59
ATOM	5675	CZ	ARG	B	365	-3.984	-3.707	40.434	1.00	40.64
ATOM	5676	NH1	ARG	B	365	-2.678	-3.913	40.385	1.00	41.51
ATOM	5677	NH2	ARG	B	365	-4.698	-4.247	41.418	1.00	41.53
ATOM	5678	C	ARG	B	365	-4.459	-2.492	34.648	1.00	39.32
ATOM	5679	O	ARG	B	365	-5.449	-1.961	34.150	1.00	39.51
ATOM	5680	N	LEU	B	366	-4.267	-3.801	34.609	1.00	41.59
ATOM	5681	CA	LEU	B	366	-5.272	-4.665	33.996	1.00	44.25
ATOM	5682	CB	LEU	B	366	-4.615	-5.908	33.366	1.00	45.24
ATOM	5683	CG	LEU	B	366	-3.640	-5.701	32.202	1.00	45.46
ATOM	5684	CD1	LEU	B	366	-4.331	-5.029	31.031	1.00	47.09
ATOM	5685	CD2	LEU	B	366	-2.489	-4.856	32.678	1.00	46.71
ATOM	5686	C	LEU	B	366	-6.263	-5.080	35.092	1.00	45.55
ATOM	5687	O	LEU	B	366	-6.424	-6.296	35.333	1.00	46.32
ATOM	5688	OXT	LEU	B	366	-6.868	-4.169	35.704	1.00	46.33
ATOM	5689	CB	ARG	C	10	-5.663	0.205	32.737	0.76	34.47
ATOM	5690	CG	ARG	C	10	-7.073	-0.397	32.771	0.76	36.85
ATOM	5691	CD	ARG	C	10	-7.748	-0.383	31.408	0.76	39.56
ATOM	5692	NE	ARG	C	10	-8.728	-1.462	31.268	0.76	41.14
ATOM	5693	CZ	ARG	C	10	-9.992	-1.301	30.875	0.76	41.65
ATOM	5694	NH1	ARG	C	10	-10.464	-0.093	30.582	0.76	41.65
ATOM	5695	NH2	ARG	C	10	-10.779	-2.365	30.749	0.76	42.22
ATOM	5696	C	ARG	C	10	-4.106	2.152	32.497	0.76	29.83
ATOM	5697	O	ARG	C	10	-3.278	1.863	33.369	0.76	26.71
ATOM	5698	N	ARG	C	10	-6.417	2.186	33.464	0.76	33.45
ATOM	5699	CA	ARG	C	10	-5.587	1.727	32.625	0.76	31.94
ATOM	5700	N	GLN	C	11	-3.805	2.853	32.408	0.76	28.04
ATOM	5701	CA	GLN	C	11	-2.458	3.321	31.094	0.76	25.66
ATOM	5702	CB	GLN	C	11	-2.423	3.866	29.662	0.76	24.07
ATOM	5703	CG	GLN	C	11	-1.047	4.361	29.231	0.76	21.39
ATOM	5704	CD	GLN	C	11	-0.039	3.245	29.174	0.76	22.59
ATOM	5705	OE1	GLN	C	11	-0.263	2.232	28.494	0.76	19.54
ATOM	5706	NE2	GLN	C	11	1.082	3.415	29.876	0.76	21.15
ATOM	5707	C	GLN	C	11	-1.895	4.396	32.038	0.76	25.33
ATOM	5708	O	GLN	C	11	-2.494	5.467	32.217	0.76	25.97
ATOM	5709	N	LEU	C	12	-0.732	4.111	32.618	0.76	24.73
ATOM	5710	CA	LEU	C	12	-0.065	5.046	33.519	0.76	25.25
ATOM	5711	CB	LEU	C	12	0.754	4.277	34.561	0.76	24.93
ATOM	5712	CG	LEU	C	12	-0.036	3.305	35.450	0.76	23.68
ATOM	5713	CD1	LEU	C	12	0.907	2.681	36.468	0.76	25.75
ATOM	5714	CD2	LEU	C	12	-1.184	4.040	36.153	0.76	25.66
ATOM	5715	C	LEU	C	12	0.845	5.948	32.680	0.76	25.12
ATOM	5716	O	LEU	C	12	1.111	5.653	31.510	0.76	25.73
ATOM	5717	N	VAL	C	13	1.317	7.044	33.273	0.76	25.64
ATOM	5718	CA	VAL	C	13	2.166	7.987	32.543	0.76	25.65
ATOM	5719	CB	VAL	C	13	1.473	9.371	32.386	0.76	26.39
ATOM	5720	CG1	VAL	C	13	0.217	9.239	31.523	0.76	26.34
ATOM	5721	CG2	VAL	C	13	1.113	9.929	33.750	0.76	26.38
ATOM	5722	C	VAL	C	13	3.542	8.211	33.174	0.76	26.02
ATOM	5723	O	VAL	C	13	3.740	8.050	34.381	0.76	24.85
ATOM	5724	N	LEU	C	14	4.498	8.596	32.339	0.76	26.90
ATOM	5725	CA	LEU	C	14	5.860	8.846	32.803	0.76	28.40
ATOM	5726	CB	LEU	C	14	6.836	8.819	31.619	0.76	28.31
ATOM	5727	CG	LEU	C	14	6.972	7.481	30.889	0.76	29.36
ATOM	5728	CD1	LEU	C	14	7.666	7.705	29.557	0.76	30.19
ATOM	5729	CD2	LEU	C	14	7.744	6.495	31.769	0.76	29.17
ATOM	5730	C	LEU	C	14	6.010	10.186	33.517	0.76	29.12
ATOM	5731	O	LEU	C	14	5.238	11.126	33.284	0.76	29.91
ATOM	5732	N	GLY	C	15	7.000	10.263	34.396	0.76	29.70
ATOM	5733	CA	GLY	C	15	7.264	11.510	35.090	0.76	32.11
ATOM	5734	C	GLY	C	15	8.263	12.275	34.234	0.76	33.78
ATOM	5735	O	GLY	C	15	9.472	12.210	34.462	0.76	35.30
ATOM	5736	N	LEU	C	16	7.750	12.995	33.241	0.76	34.34
ATOM	5737	CA	LEU	C	16	8.576	13.756	32.306	0.76	34.95
ATOM	5738	CB	LEU	C	16	7.732	14.157	31.094	0.76	33.39
ATOM	5739	CG	LEU	C	16	7.258	12.955	30.269	0.76	30.69
ATOM	5740	CD1	LEU	C	16	6.303	13.411	29.171	0.76	30.83
ATOM	5741	CD2	LEU	C	16	8.467	12.333	29.690	0.76	31.29
ATOM	5742	C	LEU	C	16	9.263	14.982	32.898	0.76	36.04
ATOM	5743	O	LEU	C	16	10.182	15.515	32.231	0.76	36.84
ATOM	5744	OXT	LEU	C	16	8.870	15.398	34.009	0.76	37.64
ATOM	5745	OH1	TIP	S	1	4.929	-23.609	18.052	1.00	15.99
ATOM	5746	OH2	TIP	S	2	4.228	8.274	-26.027	1.00	13.10
ATOM	5747	OH2	TIP	S	3	10.558	12.623	-25.084	1.00	15.30
ATOM	5748	OH2	TIP	S	4	5.227	-21.550	19.916	1.00	15.79
ATOM	5749	OH2	TIP	S	5	8.098	19.305	-28.222	1.00	16.24
ATOM	5750	OH2	TIP	S	6	15.241	27.169	-6.212	1.00	15.04
ATOM	5751	OH2	TIP	S	7	20.667	23.747	-19.701	1.00	12.11
ATOM	5752	OH2	TIP	S	8	8.057	-16.814	20.553	1.00	18.56
ATOM	5753	OH2	TIP	S	9	-8.202	-7.752	-28.805	1.00	15.40
ATOM	5754	OH2	TIP	S	10	-3.188	14.555	-36.202	1.00	15.80
ATOM	5755	OH2	TIP	S	11	-8.735	18.253	-21.735	1.00	16.46
ATOM	5756	OH2	TIP	S	12	1.707	0.243	28.691	1.00	19.43
ATOM	5757	OH2	TIP	S	13	21.827	20.941	-18.878	1.00	15.07
ATOM	5758	OH2	TIP	S	14	-12.919	1.529	-20.565	1.00	14.60
ATOM	5759	OH2	TIP	S	15	6.506	7.845	-24.491	1.00	14.11
ATOM	5760	OH2	TIP	S	16	-16.095	-26.586	6.640	1.00	18.29
ATOM	5761	OH2	TIP	S	17	-20.810	-5.324	-15.729	1.00	15.06
ATOM	5762	OH2	TIP	S	18	6.790	-16.969	34.740	1.00	14.72
ATOM	5763	OH2	TIP	S	19	-28.633	-22.763	-19.122	1.00	19.48
ATOM	5764	OH2	TIP	S	20	-4.575	19.633	-14.656	1.00	16.85
ATOM	5765	OH2	TIP	S	21	6.941	2.131	23.109	1.00	18.16

Figure 1 (continued 58)

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ATOM	5766	OH2	TIP	S	22	-27.660	-14.486	-13.561	1.00	17.12	S
ATOM	5767	OH2	TIP	S	23	-13.962	-0.925	-21.605	1.00	14.22	S
ATOM	5768	OH2	TIP	S	24	1.435	28.503	-10.938	1.00	18.48	S
ATOM	5769	OH2	TIP	S	25	9.366	3.813	23.519	1.00	16.22	S
ATOM	5770	OH2	TIP	S	26	6.434	-22.228	22.332	1.00	19.93	S
ATOM	5771	OH2	TIP	S	27	7.890	-18.056	18.119	1.00	19.57	S
ATOM	5772	OH2	TIP	S	28	-15.000	8.720	-22.814	1.00	14.68	S
ATOM	5773	OH2	TIP	S	29	10.776	24.804	-24.045	1.00	16.80	S
ATOM	5774	OH2	TIP	S	30	1.778	20.791	-6.653	1.00	17.56	S
ATOM	5775	OH2	TIP	S	31	0.621	20.501	-9.333	1.00	18.49	S
ATOM	5776	OH2	TIP	S	32	4.572	1.385	-28.353	1.00	18.53	S
ATOM	5777	OH2	TIP	S	33	8.530	13.438	21.012	1.00	18.38	S
ATOM	5778	OH2	TIP	S	34	-5.364	-34.951	13.172	1.00	16.54	S
ATOM	5779	OH2	TIP	S	35	-0.215	-6.534	-30.846	1.00	17.23	S
ATOM	5780	OH2	TIP	S	36	3.783	18.454	-29.707	1.00	19.51	S
ATOM	5781	OH2	TIP	S	37	3.591	-1.199	-27.445	1.00	19.45	S
ATOM	5782	OH2	TIP	S	38	9.369	34.981	-11.888	1.00	20.02	S
ATOM	5783	OH2	TIP	S	39	10.133	-20.154	36.900	1.00	17.90	S
ATOM	5784	OH2	TIP	S	40	3.793	8.403	-19.080	1.00	16.65	S
ATOM	5785	OH2	TIP	S	41	10.939	4.680	14.536	1.00	18.20	S
ATOM	5786	OH2	TIP	S	42	8.076	12.297	-25.798	1.00	16.16	S
ATOM	5787	OH2	TIP	S	43	-14.372	-32.728	6.563	1.00	18.38	S
ATOM	5788	OH2	TIP	S	44	-23.715	-9.227	-23.646	1.00	21.11	S
ATOM	5789	OH2	TIP	S	45	20.825	28.255	-9.159	1.00	16.67	S
ATOM	5790	OH2	TIP	S	46	-1.109	13.957	-40.824	1.00	17.50	S
ATOM	5791	OH2	TIP	S	47	5.330	-27.571	17.233	1.00	20.27	S
ATOM	5792	OH2	TIP	S	48	-6.283	-7.101	26.866	1.00	19.83	S
ATOM	5793	OH2	TIP	S	49	-4.904	-9.220	29.033	1.00	18.63	S
ATOM	5794	OH2	TIP	S	50	6.596	25.027	-2.197	1.00	18.25	S
ATOM	5795	OH2	TIP	S	51	3.946	-28.513	19.328	1.00	22.98	S
ATOM	5796	OH2	TIP	S	52	18.496	30.057	13.872	1.00	21.35	S
ATOM	5797	OH2	TIP	S	53	14.476	13.406	-26.031	1.00	20.88	S
ATOM	5798	OH2	TIP	S	54	-5.854	17.119	-30.322	1.00	18.67	S
ATOM	5799	OH2	TIP	S	55	-11.444	-12.723	13.885	1.00	21.78	S
ATOM	5800	OH2	TIP	S	56	-18.531	-23.945	-2.069	1.00	20.92	S
ATOM	5801	OH2	TIP	S	57	8.793	-1.749	36.685	1.00	23.51	S
ATOM	5802	OH2	TIP	S	58	-10.518	17.199	-18.634	1.00	19.66	S
ATOM	5803	OH2	TIP	S	59	18.320	33.650	-11.778	1.00	23.35	S
ATOM	5804	OH2	TIP	S	60	3.811	10.767	-14.624	1.00	21.33	S
ATOM	5805	OH2	TIP	S	61	10.630	-17.965	40.549	1.00	20.18	S
ATOM	5806	OH3	TIP	S	62	7.563	12.545	-28.560	1.00	22.05	S
ATOM	5807	OH2	TIP	S	63	17.504	24.804	2.515	1.00	17.88	S
ATOM	5808	OH2	TIP	S	64	11.187	4.750	-21.381	1.00	18.39	S
ATOM	5809	OH2	TIP	S	65	3.669	23.465	0.736	1.00	20.78	S
ATOM	5810	OH2	TIP	S	66	0.642	-25.439	24.271	1.00	19.92	S
ATOM	5811	OH2	TIP	S	67	-5.697	-28.454	21.972	1.00	20.88	S
ATOM	5812	OH2	TIP	S	68	4.514	12.181	-28.340	1.00	18.14	S
ATOM	5813	OH2	TIP	S	69	-20.340	-23.019	19.925	1.00	21.76	S
ATOM	5814	OH2	TIP	S	70	1.000	-3.521	35.944	1.00	23.02	S
ATOM	5815	OH2	TIP	S	71	4.561	34.315	-12.922	1.00	19.38	S
ATOM	5816	OH2	TIP	S	72	-20.556	2.785	-36.420	1.00	27.46	S
ATOM	5817	OH2	TIP	S	73	4.764	-1.117	-32.012	1.00	27.35	S
ATOM	5818	OH2	TIP	S	74	-20.786	-26.799	16.978	1.00	21.37	S
ATOM	5819	OH2	TIP	S	75	30.423	23.473	16.248	1.00	26.87	S
ATOM	5820	OH2	TIP	S	76	-14.523	15.544	-36.291	1.00	26.66	S
ATOM	5821	OH3	TIP	S	77	27.307	15.098	1.258	1.00	25.86	S
ATOM	5822	OH2	TIP	S	78	5.319	7.976	-31.697	1.00	23.44	S
ATOM	5823	OH2	TIP	S	79	8.457	-24.862	15.056	1.00	27.61	S
ATOM	5824	OH2	TIP	S	80	-0.400	-9.335	16.470	1.00	23.64	S
ATOM	5825	OH2	TIP	S	81	-30.824	-24.685	-8.816	1.00	23.87	S
ATOM	5826	OH2	TIP	S	82	-2.412	16.657	-12.786	1.00	22.67	S
ATOM	5827	OH2	TIP	S	83	-16.348	6.876	-33.518	1.00	20.01	S
ATOM	5828	OH2	TIP	S	84	4.781	13.922	-43.086	1.00	19.96	S
ATOM	5829	OH2	TIP	S	85	22.867	14.713	-4.352	1.00	27.67	S
ATOM	5830	OH2	TIP	S	86	14.019	34.958	-17.016	1.00	24.03	S
ATOM	5831	OH2	TIP	S	87	-22.863	-7.339	-7.089	1.00	30.51	S
ATOM	5832	OH2	TIP	S	88	0.014	-13.197	13.132	1.00	24.07	S
ATOM	5833	OH2	TIP	S	89	-0.477	-26.421	26.641	1.00	22.63	S
ATOM	5834	OH2	TIP	S	90	8.749	0.467	15.868	1.00	29.65	S
ATOM	5835	OH2	TIP	S	91	-6.197	-6.594	19.747	1.00	23.37	S
ATOM	5836	OH2	TIP	S	92	7.703	5.467	-24.148	1.00	20.70	S
ATOM	5837	OH2	TIP	S	93	1.486	-22.220	27.625	1.00	23.06	S
ATOM	5838	OH2	TIP	S	94	-8.748	-9.800	20.699	1.00	22.04	S
ATOM	5839	OH2	TIP	S	95	-16.624	1.189	-13.898	1.00	21.62	S
ATOM	5840	OH2	TIP	S	96	-17.781	-3.404	-34.492	1.00	24.71	S
ATOM	5841	OH2	TIP	S	97	22.028	14.095	-22.382	1.00	22.02	S
ATOM	5842	OH2	TIP	S	98	0.850	24.987	-25.136	1.00	29.29	S
ATOM	5843	OH2	TIP	S	99	3.761	-8.089	41.138	1.00	24.22	S
ATOM	5844	OH2	TIP	S	100	6.060	-19.622	23.723	1.00	20.71	S
ATOM	5845	OH2	TIP	S	101	-20.830	-8.439	-5.124	1.00	25.02	S
ATOM	5846	OH2	TIP	S	102	-23.978	-22.857	-27.649	1.00	27.37	S
ATOM	5847	OH2	TIP	S	103	-19.110	-26.350	4.119	1.00	28.04	S
ATOM	5848	OH2	TIP	S	104	-10.419	10.168	-16.512	1.00	20.89	S
ATOM	5849	OH2	TIP	S	106	-26.620	6.278	5.868	1.00	26.84	S
ATOM	5850	OH2	TIP	S	107	15.079	-16.710	41.044	1.00	31.49	S
ATOM	5851	OH2	TIP	S	108	-6.608	-4.481	27.748	1.00	21.60	S
ATOM	5852	OH2	TIP	S	109	-10.514	-6.785	27.903	1.00	28.76	S
ATOM	5853	OH2	TIP	S	110	7.483	34.057	-13.520	1.00	20.71	S
ATOM	5854	OH2	TIP	S	111	-6.501	-31.759	-5.806	1.00	31.23	S
ATOM	5855	OH2	TIP	S	112	-2.508	-7.957	17.238	1.00	28.35	S
ATOM	5856	OH2	TIP	S	113	-16.554	3.360	-34.120	1.00	19.83	S
ATOM	5857	OH2	TIP	S	114	-1.472	10.711	-15.764	1.00	27.87	S
ATOM	5858	OH2	TIP	S	115	-22.960	-28.887	-19.727	1.00	25.60	S
ATOM	5859	OH2	TIP	S	116	15.115	-14.901	19.731	1.00	24.51	S
ATOM	5860	OH2	TIP	S	117	-5.148	-33.100	-3.606	1.00	25.41	S
ATOM	5861	OH2	TIP	S	118	20.099	-0.396	23.402	1.00	22.68	S
ATOM	5862	OH2	TIP	S	119	-7.111	-2.117	-16.703	1.00	24.27	S
ATOM	5863	OH2	TIP	S	120	-11.193	-9.224	19.755	1.00	25.30	S
ATOM	5864	OH2	TIP	S	121	18.193	-11.449	36.973	1.00	27.57	S
ATOM	5865	OH2	TIP	S	122	-22.357	2.771	-13.647	1.00	25.49	S

Figure 1 (continued 59)

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ATOM	5866	OH2	TIP	S	123	20.077	32.381	13.831	1.00	28.68	S
ATOM	5867	OH2	TIP	S	124	-17.741	4.784	-15.367	1.00	27.89	S
ATOM	5868	OH2	TIP	S	125	4.106	-14.005	15.492	1.00	25.37	S
ATOM	5869	OH2	TIP	S	126	13.838	16.125	-26.991	1.00	25.20	S
ATOM	5870	OH2	TIP	S	127	-2.287	-34.498	8.522	1.00	26.09	S
ATOM	5871	OH2	TIP	S	128	-11.663	-6.092	22.298	1.00	28.13	S
ATOM	5872	OH2	TIP	S	129	11.561	18.821	-28.755	1.00	36.46	S
ATOM	5873	OH2	TIP	S	130	7.031	1.863	-26.963	1.00	26.76	S
ATOM	5874	OH2	TIP	S	131	6.205	-28.726	8.902	1.00	29.30	S
ATOM	5875	OH2	TIP	S	132	-10.559	19.568	-19.983	1.00	20.77	S
ATOM	5876	OH2	TIP	S	133	22.972	19.220	-17.034	1.00	20.45	S
ATOM	5877	OH2	TIP	S	134	5.249	21.787	8.628	1.00	29.10	S
ATOM	5878	OH2	TIP	S	135	16.410	14.232	27.045	1.00	27.03	S
ATOM	5879	OH2	TIP	S	136	-3.218	-34.687	11.046	1.00	24.07	S
ATOM	5880	OH2	TIP	S	137	24.833	28.261	-21.884	1.00	22.96	S
ATOM	5881	OH2	TIP	S	138	13.264	35.476	-14.774	1.00	30.23	S
ATOM	5882	OH2	TIP	S	139	-2.053	2.392	26.549	1.00	25.03	S
ATOM	5883	OH2	TIP	S	140	11.605	15.067	0.133	1.00	34.22	S
ATOM	5884	OH2	TIP	S	141	13.972	24.010	19.832	1.00	25.81	S
ATOM	5885	OH2	TIP	S	142	-13.355	-25.503	19.026	1.00	29.46	S
ATOM	5886	OH2	TIP	S	143	-4.006	-31.965	2.763	1.00	26.41	S
ATOM	5887	OH2	TIP	S	144	15.901	28.652	-2.514	1.00	25.23	S
ATOM	5888	OH2	TIP	S	145	-17.355	-32.497	18.572	1.00	25.07	S
ATOM	5889	OH2	TIP	S	146	0.958	-13.688	32.466	1.00	22.13	S
ATOM	5890	OH2	TIP	S	147	-6.459	12.128	-44.255	1.00	32.10	S
ATOM	5891	OH2	TIP	S	148	-0.707	-24.653	2.977	1.00	26.54	S
ATOM	5892	OH2	TIP	S	149	-12.838	-12.951	11.427	1.00	23.90	S
ATOM	5893	OH2	TIP	S	150	-24.404	-11.780	-24.495	1.00	25.54	S
ATOM	5894	OH2	TIP	S	151	0.539	-6.289	-33.601	1.00	29.88	S
ATOM	5895	OH2	TIP	S	152	-13.161	-28.396	-0.606	1.00	27.46	S
ATOM	5896	OH2	TIP	S	153	10.877	9.824	5.701	1.00	24.98	S
ATOM	5897	OH2	TIP	S	154	-24.429	-25.832	1.553	1.00	29.48	S
ATOM	5898	OH2	TIP	S	155	9.976	29.261	3.159	1.00	26.39	S
ATOM	5899	OH2	TIP	S	156	-8.594	-7.245	-13.161	1.00	38.12	S
ATOM	5900	OH2	TIP	S	157	2.066	24.920	5.025	1.00	22.77	S
ATOM	5901	OH2	TIP	S	158	-15.909	14.296	-28.353	1.00	25.22	S
ATOM	5902	OH2	TIP	S	159	0.091	16.467	-11.319	1.00	24.31	S
ATOM	5903	OH2	TIP	S	160	16.526	-12.797	18.583	1.00	26.81	S
ATOM	5904	OH2	TIP	S	161	3.049	7.864	19.831	1.00	24.57	S
ATOM	5905	OH2	TIP	S	162	21.865	-8.253	21.271	1.00	23.66	S
ATOM	5906	OH2	TIP	S	163	-7.960	-6.892	-33.834	1.00	30.32	S
ATOM	5907	OH2	TIP	S	164	19.362	-16.854	36.055	1.00	31.05	S
ATOM	5908	OH2	TIP	S	165	-5.308	-32.390	18.952	1.00	29.57	S
ATOM	5909	OH2	TIP	S	166	-11.933	-29.026	-5.229	1.00	26.58	S
ATOM	5910	OH2	TIP	S	167	-19.093	-31.089	17.480	1.00	33.54	S
ATOM	5911	OH2	TIP	S	168	14.092	18.448	-25.956	1.00	29.46	S
ATOM	5912	OH2	TIP	S	169	10.876	5.438	12.054	1.00	32.82	S
ATOM	5913	OH2	TIP	S	170	-6.890	-9.072	-26.532	1.00	25.82	S
ATOM	5914	OH2	TIP	S	171	29.867	28.203	18.182	1.00	30.29	S
ATOM	5915	OH2	TIP	S	172	16.406	39.004	9.209	1.00	28.96	S
ATOM	5916	OH2	TIP	S	173	-4.013	-11.245	30.748	1.00	25.90	S
ATOM	5917	OH2	TIP	S	174	-26.979	-31.890	-8.368	1.00	36.88	S
ATOM	5918	OH2	TIP	S	175	-23.390	1.597	-33.916	1.00	36.95	S
ATOM	5919	OH2	TIP	S	176	-21.827	-20.068	21.374	1.00	28.64	S
ATOM	5920	OH2	TIP	S	177	-17.123	-16.612	7.118	1.00	25.01	S
ATOM	5921	OH2	TIP	S	178	-0.586	30.510	-11.769	1.00	23.24	S
ATOM	5922	OH2	TIP	S	179	6.159	20.259	17.337	1.00	30.73	S
ATOM	5923	OH2	TIP	S	180	21.260	-1.762	19.163	1.00	34.09	S
ATOM	5924	OH2	TIP	S	181	-2.864	-28.282	2.753	1.00	27.53	S
ATOM	5925	OH2	TIP	S	182	-8.835	-11.179	-6.743	1.00	29.61	S
ATOM	5926	OH2	TIP	S	183	15.829	24.884	-23.368	1.00	31.33	S
ATOM	5927	OH2	TIP	S	184	24.002	17.831	-10.733	1.00	29.65	S
ATOM	5928	OH2	TIP	S	185	-29.401	5.440	-14.949	1.00	32.48	S
ATOM	5929	OH2	TIP	S	186	-1.383	-33.459	19.317	1.00	29.25	S
ATOM	5930	OH2	TIP	S	187	12.063	-19.966	25.080	1.00	25.65	S
ATOM	5931	OH2	TIP	S	188	-4.351	-9.679	-26.788	1.00	27.17	S
ATOM	5932	OH2	TIP	S	189	3.729	5.832	16.486	1.00	34.24	S
ATOM	5933	OH2	TIP	S	190	9.565	37.434	-9.975	1.00	27.30	S
ATOM	5934	OH2	TIP	S	191	1.483	14.975	-40.508	1.00	31.36	S
ATOM	5935	OH2	TIP	S	192	-6.648	-10.961	-20.165	1.00	32.28	S
ATOM	5936	OH2	TIP	S	193	3.745	12.221	31.113	1.00	29.48	S
ATOM	5937	OH2	TIP	S	194	2.400	-29.701	-15.849	1.00	26.51	S
ATOM	5938	OH2	TIP	S	195	1.145	-29.287	18.977	1.00	27.97	S
ATOM	5939	OH2	TIP	S	196	1.173	24.321	-30.127	1.00	37.69	S
ATOM	5940	OH2	TIP	S	197	-28.254	-20.580	5.716	1.00	43.95	S
ATOM	5941	OH2	TIP	S	198	22.283	20.039	25.715	1.00	34.76	S
ATOM	5942	OH2	TIP	S	199	-1.895	4.664	-43.775	1.00	27.75	S
ATOM	5943	OH2	TIP	S	200	23.429	31.198	-15.860	1.00	32.99	S
ATOM	5944	OH2	TIP	S	201	-9.479	-5.901	-15.419	1.00	21.16	S
ATOM	5945	OH2	TIP	S	202	-12.878	0.162	-12.723	1.00	-33.84	S
ATOM	5946	OH2	TIP	S	203	5.581	19.187	14.793	1.00	27.97	S
ATOM	5947	OH2	TIP	S	204	-23.954	-24.578	-2.262	1.00	30.51	S
ATOM	5948	OH2	TIP	S	205	3.457	33.211	-23.268	1.00	31.98	S
ATOM	5949	OH2	TIP	S	206	-17.263	0.457	-42.268	1.00	31.49	S
ATOM	5950	OH2	TIP	S	207	16.260	31.888	2.413	1.00	23.24	S
ATOM	5951	OH2	TIP	S	208	-4.320	1.145	26.565	1.00	29.38	S
ATOM	5952	OH2	TIP	S	209	-19.947	2.160	-11.744	1.00	38.41	S
ATOM	5953	OH2	TIP	S	210	1.872	26.689	-27.041	1.00	29.78	S
ATOM	5954	OH2	TIP	S	211	-13.714	23.099	-13.845	1.00	33.77	S
ATOM	5955	OH2	TIP	S	212	9.218	35.580	-19.331	1.00	29.22	S
ATOM	5956	OH2	TIP	S	213	-0.219	26.259	5.173	1.00	31.76	S
ATOM	5957	OH2	TIP	S	214	-8.272	3.938	-13.966	1.00	35.25	S
ATOM	5958	OH2	TIP	S	215	9.984	-22.548	31.867	1.00	33.85	S
ATOM	5959	OH2	TIP	S	216	-30.186	-28.425	2.476	1.00	30.05	S
ATOM	5960	OH2	TIP	S	217	5.272	16.545	-36.105	1.00	33.10	S
ATOM	5961	OH2	TIP	S	218	-14.957	-2.170	-39.231	1.00	30.96	S
ATOM	5962	OH2	TIP	S	219	2.136	-28.846	23.097	1.00	39.83	S
ATOM	5963	OH2	TIP	S	220	0.866	11.873	23.871	1.00	32.14	S
ATOM	5964	OH2	TIP	S	221	-7.469	-8.003	-23.367	1.00	24.79	S
ATOM	5965	OH2	TIP	S	222	10.219	6.251	34.646	1.00	37.06	S

Figure 1 (continued 60)

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ATOM	5966	OH2	TIP	S	223	9.603	-19.191	12.099	1.00	30.03
ATOM	5967	OH2	TIP	S	224	15.592	1.270	14.898	1.00	29.33
ATOM	5968	OH2	TIP	S	225	-7.625	-22.611	-22.802	1.00	32.63
ATOM	5969	OH2	TIP	S	226	-30.236	-24.968	-11.543	1.00	24.51
ATOM	5970	OH2	TIP	S	227	-11.748	-27.136	28.999	1.00	35.80
ATOM	5971	OH2	TIP	S	228	-17.912	-19.364	23.072	1.00	31.69
ATOM	5972	OH2	TIP	S	229	-12.001	4.279	-15.335	1.00	28.59
ATOM	5973	OH2	TIP	S	230	27.573	31.316	11.831	1.00	32.14
ATOM	5974	OH2	TIP	S	231	-25.350	3.037	-21.957	1.00	30.50
ATOM	5975	OH2	TIP	S	232	-9.948	19.698	-27.138	1.00	32.26
ATOM	5976	OH2	TIP	S	233	31.351	11.309	12.566	1.00	40.60
ATOM	5977	OH2	TIP	S	234	7.345	8.147	-8.973	1.00	40.15
ATOM	5978	OH2	TIP	S	235	13.323	25.650	-24.378	1.00	28.39
ATOM	5979	OH2	TIP	S	236	14.326	-23.002	38.347	1.00	44.20
ATOM	5980	OH2	TIP	S	237	18.205	35.226	-19.376	1.00	36.69
ATOM	5981	OH2	TIP	S	238	7.073	7.343	-21.458	1.00	26.18
ATOM	5982	OH2	TIP	S	239	6.134	-17.380	11.852	1.00	34.32
ATOM	5983	OH2	TIP	S	240	-6.807	3.536	-42.001	1.00	25.28
ATOM	5984	OH2	TIP	S	241	-24.937	-17.863	-25.603	1.00	32.04
ATOM	5985	OH2	TIP	S	242	-17.088	-21.664	-30.797	1.00	30.50
ATOM	5986	OH2	TIP	S	243	6.771	-7.663	14.406	1.00	36.01
ATOM	5987	OH2	TIP	S	244	-27.706	-30.578	-5.708	1.00	47.96
ATOM	5988	OH2	TIP	S	245	-21.059	10.316	-25.562	1.00	35.65
ATOM	5989	OH2	TIP	S	246	10.606	28.216	-25.525	1.00	29.43
ATOM	5990	OH2	TIP	S	247	1.528	5.171	-17.593	1.00	27.85
ATOM	5991	OH2	TIP	S	248	-29.012	-18.667	-20.134	1.00	33.27
ATOM	5992	OH2	TIP	S	249	-21.413	-24.797	-4.888	1.00	34.44
ATOM	5993	OH2	TIP	S	250	1.196	-8.297	-29.245	1.00	27.57
ATOM	5994	OH2	TIP	S	251	-0.162	-13.772	35.108	1.00	36.60
ATOM	5995	OH2	TIP	S	252	19.156	-15.454	21.696	1.00	29.04
ATOM	5996	OH2	TIP	S	253	21.723	17.101	-18.745	1.00	9.13
ATOM	5997	OH2	TIP	S	254	7.667	9.573	-26.321	1.00	15.05
ATOM	5998	OH2	TIP	S	255	5.459	9.537	-28.155	1.00	14.20
ATOM	5999	OH2	TIP	S	256	7.583	-20.372	19.535	1.00	17.45
ATOM	6000	OH2	TIP	S	257	8.434	5.091	-21.601	1.00	20.19
ATOM	6001	OH2	TIP	S	258	10.303	-20.727	39.479	1.00	21.19
ATOM	6002	OH2	TIP	S	259	23.351	15.777	-20.932	1.00	24.25
ATOM	6003	OH2	TIP	S	260	8.255	-19.223	21.937	1.00	16.91
ATOM	6004	OH2	TIP	S	261	7.407	21.555	-29.683	1.00	18.42
ATOM	6005	OH2	TIP	S	262	0.133	-33.614	9.571	1.00	23.67
ATOM	6006	OH2	TIP	S	263	1.067	23.311	-27.412	1.00	26.04
ATOM	6007	OH2	TIP	S	264	10.172	-20.657	23.070	1.00	20.75
ATOM	6008	OH2	TIP	S	265	5.434	1.347	-31.078	1.00	25.19
ATOM	6009	OH2	TIP	S	266	6.473	8.791	-30.462	1.00	22.73
ATOM	6010	OH2	TIP	S	267	16.690	-16.534	21.428	1.00	26.86
ATOM	6011	OH2	TIP	S	268	-7.886	21.056	-13.245	1.00	26.88
ATOM	6012	OH2	TIP	S	269	12.771	20.121	-27.176	1.00	33.96
ATOM	6013	OH2	TIP	S	270	-17.226	9.655	-21.614	1.00	26.62
ATOM	6014	OH2	TIP	S	271	-2.213	14.948	-43.167	1.00	24.59
ATOM	6015	OH2	TIP	S	272	9.664	5.525	-25.968	1.00	25.89
ATOM	6016	OH2	TIP	S	273	6.917	-25.402	17.512	1.00	27.80
ATOM	6017	OH2	TIP	S	274	-4.242	-20.885	28.965	1.00	32.23
ATOM	6018	OH2	TIP	S	275	-17.221	-17.062	17.975	1.00	18.09
ATOM	6019	OH2	TIP	S	276	12.668	11.417	-26.228	1.00	27.75
ATOM	6020	OH2	TIP	S	277	10.299	1.950	14.305	1.00	27.65
ATOM	6021	OH2	TIP	S	278	-31.806	-30.359	-6.948	1.00	57.47
ATOM	6022	OH2	TIP	S	279	-26.463	4.339	-9.507	1.00	29.65
ATOM	6023	OH2	TIP	S	280	-26.015	-34.574	-7.677	1.00	26.06
ATOM	6024	OH2	TIP	S	281	-31.347	5.379	-17.218	1.00	33.42
ATOM	6025	OH2	TIP	S	282	14.453	-16.744	17.668	1.00	30.41
ATOM	6026	OH2	TIP	S	283	27.710	8.976	5.055	1.00	26.81
ATOM	6027	OH2	TIP	S	284	2.896	8.795	-16.720	1.00	27.99
ATOM	6028	OH2	TIP	S	285	-9.100	19.482	-24.203	1.00	25.80
ATOM	6029	OH2	TIP	S	286	-2.579	1.667	21.500	1.00	29.60
ATOM	6030	OH2	TIP	S	287	6.335	11.378	-31.555	1.00	29.71
ATOM	6031	OH2	TIP	S	288	12.371	-16.564	41.802	1.00	31.26
ATOM	6032	OH2	TIP	S	289	0.360	-29.275	21.468	1.00	31.50
ATOM	6033	OH2	TIP	S	290	-2.645	4.725	26.240	1.00	33.72
ATOM	6034	OH2	TIP	S	291	19.718	-0.267	20.338	1.00	32.39
ATOM	6035	OH2	TIP	S	292	7.034	29.199	9.979	1.00	29.78
ATOM	6036	OH2	TIP	S	293	-4.995	20.991	-12.507	1.00	34.58
ATOM	6037	OH2	TIP	S	294	-28.086	-24.068	-26.481	1.00	30.52
ATOM	6038	OH2	TIP	S	295	4.690	32.380	-25.768	1.00	32.16
ATOM	6039	OH2	TIP	S	296	12.183	37.736	-9.852	1.00	32.44
ATOM	6040	OH2	TIP	S	297	-0.897	-9.935	-28.834	1.00	28.74
ATOM	6041	OH2	TIP	S	298	-5.666	-26.946	-3.776	1.00	35.30
ATOM	6042	OH2	TIP	S	299	-19.121	-17.609	23.997	1.00	30.20
ATOM	6043	OH2	TIP	S	300	11.846	2.521	-20.488	1.00	34.76
ATOM	6044	OH2	TIP	S	301	21.299	6.735	24.995	1.00	37.00
ATOM	6045	OH2	TIP	S	302	-23.638	-27.161	16.432	1.00	29.19
ATOM	6046	OH2	TIP	S	303	1.556	-0.845	-22.820	1.00	34.60
ATOM	6047	OH2	TIP	S	304	-12.057	-30.800	-2.592	1.00	30.84
ATOM	6048	OH2	TIP	S	305	16.694	-19.967	30.452	1.00	32.66
ATOM	6049	OH2	TIP	S	306	0.157	25.634	-7.191	1.00	32.17
ATOM	6050	OH2	TIP	S	307	-0.449	27.840	-20.073	1.00	29.18
ATOM	6051	OH2	TIP	S	308	21.819	3.025	9.910	1.00	41.68
ATOM	6052	OH2	TIP	S	309	-15.005	-11.439	-28.535	1.00	38.02
ATOM	6053	OH2	TIP	S	310	-21.942	-31.716	-8.240	1.00	33.01
ATOM	6054	OH2	TIP	S	311	-8.284	-25.125	-23.593	1.00	41.18
ATOM	6055	OH2	TIP	S	312	2.515	4.002	-33.125	1.00	26.47
ATOM	6056	OH2	TIP	S	313	-18.335	13.849	-29.235	1.00	30.43
ATOM	6057	OH2	TIP	S	314	-12.912	-8.449	21.566	1.00	30.42
ATOM	6058	OH2	TIP	S	315	-1.397	-26.362	1.310	1.00	33.91
ATOM	6059	OH2	TIP	S	316	9.366	-22.526	35.732	1.00	30.66
ATOM	6060	OH2	TIP	S	317	-25.401	-30.023	-8.998	1.00	29.44
ATOM	6061	OH2	TIP	S	318	-21.887	3.702	-34.234	1.00	36.98
ATOM	6062	OH2	TIP	S	319	-8.700	-20.782	-24.886	1.00	32.89
ATOM	6063	OH2	TIP	S	320	-20.333	-29.925	-6.872	1.00	34.64
ATOM	6064	OH2	TIP	S	321	7.827	-13.241	-33.387	1.00	32.71
ATOM	6065	OH2	TIP	S	322	14.750	31.182	9.293	1.00	31.66

Figure 1 (continued 61)

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ATOM	6066	OH2	TIP	S	323	-24.400	-19.167	20.554	1.00	30.46	S
ATOM	6067	OH2	TIP	S	324	-9.584	3.692	-42.248	1.00	33.30	S
ATOM	6068	OH2	TIP	S	325	-6.014	19.032	-31.179	1.00	40.38	S
ATOM	6069	OH2	TIP	S	326	-13.974	-30.622	-5.965	1.00	32.26	S
ATOM	6070	OH2	TIP	S	327	-22.857	-10.593	-7.579	1.00	34.80	S
ATOM	6071	OH2	TIP	S	328	12.690	33.497	-20.379	1.00	34.07	S
ATOM	6072	OH2	TIP	S	329	7.069	2.658	-20.988	1.00	28.88	S
ATOM	6073	OH2	TIP	S	330	12.019	-0.360	36.086	1.00	26.34	S
ATOM	6074	OH2	TIP	S	331	-22.705	5.938	-14.330	1.00	34.70	S
ATOM	6075	OH2	TIP	S	332	8.097	14.122	-2.649	1.00	39.46	S
ATOM	6076	OH2	TIP	S	333	-21.898	-21.927	4.044	1.00	37.81	S
ATOM	6077	OH2	TIP	S	334	9.937	-17.771	16.216	1.00	29.70	S
ATOM	6078	OH2	TIP	S	335	-16.221	-6.845	-33.678	1.00	33.31	S
ATOM	6079	OH2	TIP	S	336	-3.494	-22.898	-17.063	1.00	31.83	S
ATOM	6080	OH2	TIP	S	337	-22.157	5.573	-30.240	1.00	39.35	S
ATOM	6081	OH2	TIP	S	338	-7.617	-32.398	-8.188	1.00	30.34	S
ATOM	6082	OH2	TIP	S	339	23.475	29.150	-8.430	1.00	36.32	S
ATOM	6083	OH2	TIP	S	340	-7.276	-9.187	-35.186	1.00	41.69	S
ATOM	6084	OH2	TIP	S	341	26.845	32.870	8.481	1.00	37.63	S
ATOM	6085	OH2	TIP	S	342	-12.192	21.236	-21.321	1.00	30.21	S
ATOM	6086	OH2	TIP	S	343	-14.628	-35.461	19.832	1.00	35.16	S
ATOM	6087	OH2	TIP	S	344	-5.653	-31.128	21.101	1.00	34.25	S
ATOM	6088	OH2	TIP	S	345	-6.084	-8.172	-19.496	1.00	36.21	S
ATOM	6089	OH2	TIP	S	346	27.089	28.347	6.056	1.00	42.19	S
ATOM	6090	OH2	TIP	S	347	17.043	22.284	-26.012	1.00	32.12	S
ATOM	6091	OH2	TIP	S	348	-21.277	2.842	-26.424	1.00	36.86	S
ATOM	6092	OH2	TIP	S	349	-23.886	-14.574	-31.320	1.00	39.26	S
ATOM	6093	OH2	TIP	S	350	5.980	19.532	10.965	1.00	26.13	S
ATOM	6094	OH2	TIP	S	351	15.574	-9.666	16.201	1.00	35.41	S
ATOM	6095	OH2	TIP	S	352	-20.467	-13.308	-4.732	1.00	35.05	S
ATOM	6096	OH2	TIP	S	353	3.368	14.285	32.732	1.00	36.22	S
ATOM	6097	OH2	TIP	S	354	-7.181	18.881	-31.723	1.00	38.24	S
ATOM	6098	OH2	TIP	S	355	-28.089	-22.839	-28.744	1.00	37.10	S
ATOM	6099	OH2	TIP	S	356	20.976	15.824	-10.665	1.00	30.49	S
ATOM	6100	OH2	TIP	S	357	-28.758	-11.680	-18.762	1.00	30.24	S
ATOM	6101	OH2	TIP	S	358	7.259	27.237	24.216	1.00	43.84	S
ATOM	6102	OH2	TIP	S	359	-1.640	22.549	-9.537	1.00	31.98	S
ATOM	6103	OH2	TIP	S	360	-4.918	-24.935	-15.685	1.00	38.37	S
ATOM	6104	OH2	TIP	S	361	4.941	-2.575	16.309	1.00	33.12	S
ATOM	6105	OH2	TIP	S	362	9.096	-17.304	13.805	1.00	34.53	S
ATOM	6106	OH2	TIP	S	363	-5.045	-8.870	15.785	1.00	34.10	S
ATOM	6107	OH2	TIP	S	364	17.874	2.521	14.615	1.00	31.53	S
ATOM	6108	OH2	TIP	S	365	-10.159	-16.244	-28.446	1.00	34.86	S
ATOM	6109	OH2	TIP	S	366	4.946	7.818	-15.134	1.00	35.25	S
ATOM	6110	OH2	TIP	S	367	-6.685	-11.153	14.460	1.00	34.00	S
ATOM	6111	OH2	TIP	S	368	14.487	-20.336	24.009	1.00	40.57	S
ATOM	6112	OH2	TIP	S	369	-1.563	6.524	-45.958	1.00	34.28	S
ATOM	6113	OH2	TIP	S	370	0.375	7.077	23.000	1.00	39.83	S
ATOM	6114	OH2	TIP	S	371	17.591	31.139	-0.347	1.00	42.33	S
ATOM	6115	OH2	TIP	S	372	-16.867	13.392	-37.376	1.00	41.73	S
ATOM	6116	OH2	TIP	S	373	-12.567	7.824	-44.159	1.00	41.23	S
ATOM	6117	OH2	TIP	S	374	26.381	23.140	-10.721	1.00	31.69	S
ATOM	6118	OH2	TIP	S	375	9.272	35.080	2.703	1.00	40.85	S
ATOM	6119	OH2	TIP	S	376	9.264	3.347	41.197	1.00	40.36	S
ATOM	6120	OH2	TIP	S	377	25.188	14.056	27.610	1.00	34.17	S
ATOM	6121	OH2	TIP	S	378	5.411	-5.742	41.987	1.00	42.27	S
ATOM	6122	OH2	TIP	S	379	-11.338	22.385	-17.862	1.00	32.59	S
ATOM	6123	OH2	TIP	S	380	-20.579	13.226	-28.071	1.00	32.84	S
ATOM	6124	OH2	TIP	S	381	8.683	9.553	3.945	1.00	34.93	S
ATOM	6125	OH2	TIP	S	382	0.828	11.135	-13.934	1.00	42.23	S
ATOM	6126	OH2	TIP	S	383	-21.600	-31.698	-19.564	1.00	38.49	S
ATOM	6127	OH2	TIP	S	384	21.597	31.274	15.485	1.00	35.82	S
ATOM	6128	OH2	TIP	S	385	12.268	35.903	4.587	1.00	31.57	S
ATOM	6129	OH2	TIP	S	386	-10.826	21.324	-11.527	1.00	38.64	S
ATOM	6130	OH2	TIP	S	387	20.994	17.489	-8.486	1.00	40.11	S
ATOM	6131	OH2	TIP	S	388	-18.148	20.285	-25.433	1.00	31.64	S
ATOM	6132	OH2	TIP	S	389	18.469	17.950	25.908	1.00	38.40	S
ATOM	6133	OH2	TIP	S	390	-17.756	2.318	-44.136	1.00	37.68	S
ATOM	6134	OH2	TIP	S	391	23.292	-5.751	18.962	1.00	37.56	S
ATOM	6135	OH2	TIP	S	392	-5.798	2.354	-16.069	1.00	37.13	S
ATOM	6136	OH2	TIP	S	393	2.260	-2.829	-24.110	1.00	34.35	S
ATOM	6137	OH2	TIP	S	394	-1.341	7.648	-12.393	1.00	33.61	S
ATOM	6138	OH2	TIP	S	395	14.575	6.039	-16.208	1.00	33.64	S
ATOM	6139	OH2	TIP	S	396	21.269	15.381	-6.817	1.00	40.16	S
ATOM	6140	OH2	TIP	S	397	11.903	28.956	0.420	1.00	35.70	S
ATOM	6141	OH2	TIP	S	398	8.524	-21.963	24.816	1.00	30.69	S
ATOM	6142	OH2	TIP	S	399	-19.214	-17.096	20.987	1.00	39.79	S
ATOM	6143	OH2	TIP	S	400	-30.167	-21.541	-5.640	1.00	38.19	S
ATOM	6144	OH2	TIP	S	401	9.901	9.176	7.979	1.00	37.49	S
ATOM	6145	OH2	TIP	S	402	-4.981	-29.566	1.767	1.00	34.27	S
ATOM	6146	OH2	TIP	S	403	22.136	13.679	-1.917	1.00	36.13	S
ATOM	6147	OH2	TIP	S	404	-13.420	-2.821	26.291	1.00	31.35	S
ATOM	6148	OH2	TIP	S	405	-21.015	-10.324	-1.067	1.00	35.17	S
ATOM	6149	OH2	TIP	S	406	4.107	-17.741	35.320	1.00	29.07	S
ATOM	6150	OH2	TIP	S	407	20.599	24.525	23.153	1.00	39.40	S
ATOM	6151	OH2	TIP	S	408	-29.430	-5.137	-24.806	1.00	31.71	S
ATOM	6152	OH2	TIP	S	409	6.574	17.571	29.465	1.00	37.78	S
ATOM	6153	OH2	TIP	S	410	25.806	21.628	-4.370	1.00	39.24	S
ATOM	6154	OH2	TIP	S	411	-18.143	-31.597	-26.039	1.00	38.21	S
ATOM	6155	OH2	TIP	S	412	-1.328	25.281	-12.054	1.00	31.58	S
ATOM	6156	OH2	TIP	S	413	0.344	10.818	20.777	1.00	42.29	S
ATOM	6157	OH2	TIP	S	414	-18.150	-29.804	-21.191	1.00	35.29	S
ATOM	6158	OH2	TIP	S	415	-23.823	-3.528	-33.040	1.00	40.40	S
ATOM	6159	OH2	TIP	S	416	1.739	1.943	19.314	1.00	36.07	S
ATOM	6160	OH2	TIP	S	417	-27.131	-17.300	-23.592	1.00	38.57	S
ATOM	6161	OH2	TIP	S	418	17.275	0.759	18.671	1.00	31.62	S
ATOM	6162	OH2	TIP	S	419	0.007	26.223	-9.446	1.00	41.38	S
ATOM	6163	OH2	TIP	S	420	-13.181	-10.416	10.475	1.00	37.29	S
ATOM	6164	OH2	TIP	S	421	-18.110	16.629	-32.614	1.00	36.54	S
ATOM	6165	OH2	TIP	S	422	7.358	26.526	17.628	1.00	39.18	S

Figure 1.(continued.62)

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ATOM	6166	OH2	TIP	S	423	17.448	-14.531	17.011	1.00	35.91	S
ATOM	6167	OH2	TIP	S	424	-10.700	-26.518	31.162	1.00	35.06	S
ATOM	6168	OH2	TIP	S	425	-9.328	-9.491	-8.639	1.00	37.90	S
ATOM	6169	OH2	TIP	S	426	-17.105	-29.156	-14.203	1.00	24.63	S
ATOM	6170	OH2	TIP	S	427	5.332	11.493	13.731	1.00	37.93	S
ATOM	6171	OH2	TIP	S	428	6.050	9.224	14.792	1.00	30.75	S
ATOM	6172	OH2	TIP	S	429	4.345	13.808	15.393	1.00	29.44	S
ATOM	6173	OH2	TIP	S	430	8.193	12.380	12.091	1.00	21.45	S
ATOM	6174	OH2	TIP	S	431	-28.556	-20.447	-15.197	1.00	37.37	S
ATOM	6175	OH2	TIP	S	432	12.135	28.679	16.661	1.00	40.91	S
ATOM	6176	OH2	TIP	S	433	6.265	25.002	25.462	1.00	33.19	S
ATOM	6177	OH2	TIP	S	434	-2.131	-25.697	31.299	1.00	31.13	S
ATOM	6178	OH2	TIP	S	435	-5.343	-20.243	26.687	1.00	32.69	S
ATOM	6179	OH2	TIP	S	436	-24.850	-28.762	-6.570	1.00	37.97	S
ATOM	6180	OH2	TIP	S	437	-22.436	0.184	-22.971	1.00	44.02	S
ATOM	6181	OH2	TIP	S	438	1.275	22.882	-25.085	1.00	48.03	S
ATOM	6182	OH2	TIP	S	439	7.058	13.884	-6.158	1.00	31.71	S
ATOM	6183	OH2	TIP	S	440	13.032	24.424	22.464	1.00	39.78	S
ATOM	6184	OH2	TIP	S	441	20.078	26.105	19.324	1.00	31.16	S
ATOM	6185	OH2	TIP	S	442	4.931	-19.598	38.096	1.00	32.92	S
ATOM	6186	OH2	TIP	S	443	-5.576	-22.456	27.255	1.00	65.54	S
ATOM	6187	OH2	TIP	S	444	22.214	-2.644	27.541	1.00	35.37	S
ATOM	6188	OH2	TIP	S	445	20.892	5.709	27.304	1.00	39.35	S
END											

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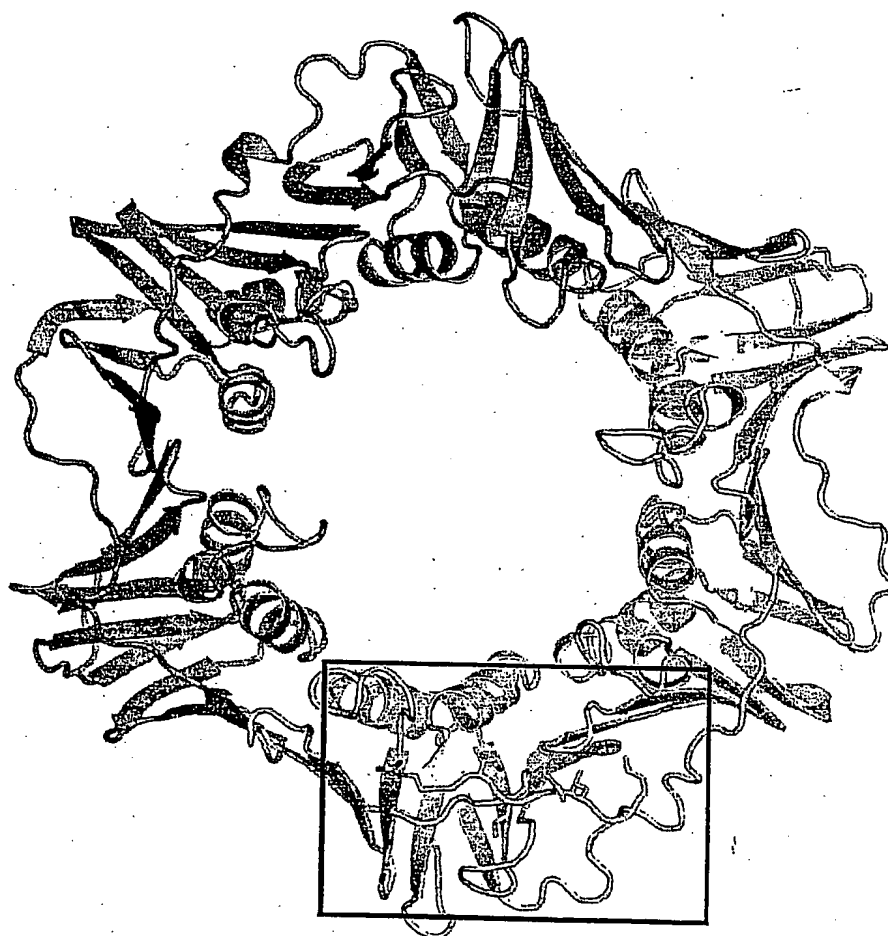


Figure 2

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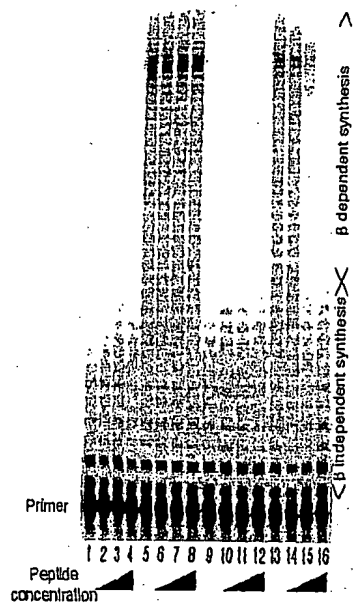


Figure 3A

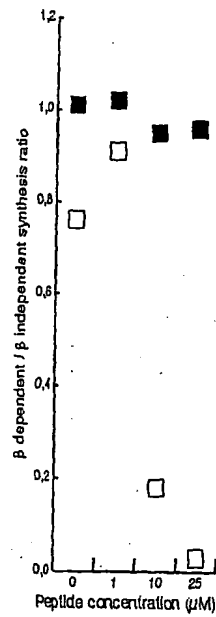


Figure 3B

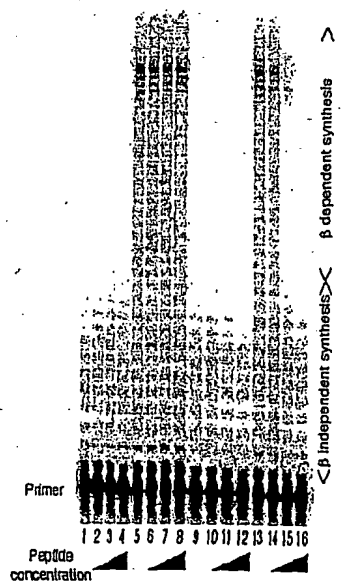


Figure 3C

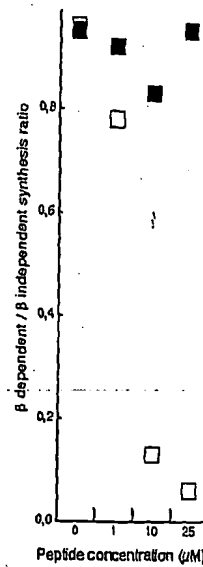


Figure 3D

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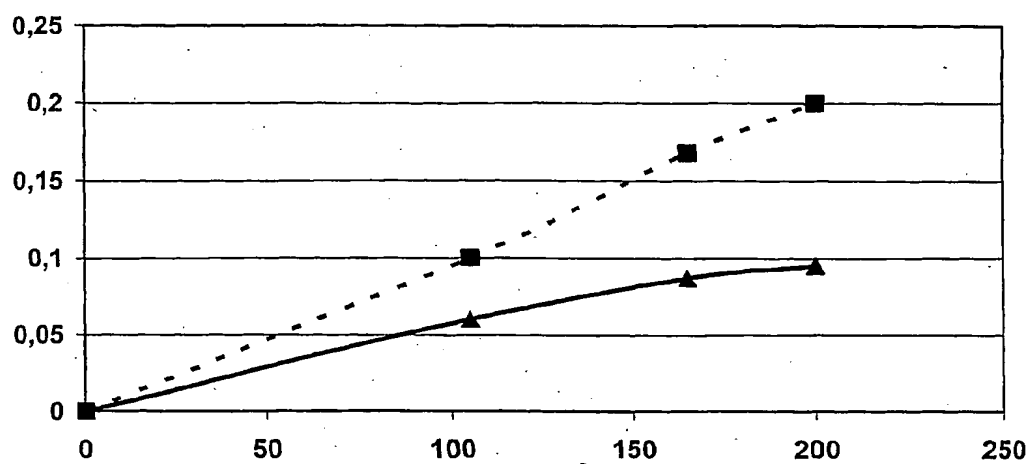


Figure 4

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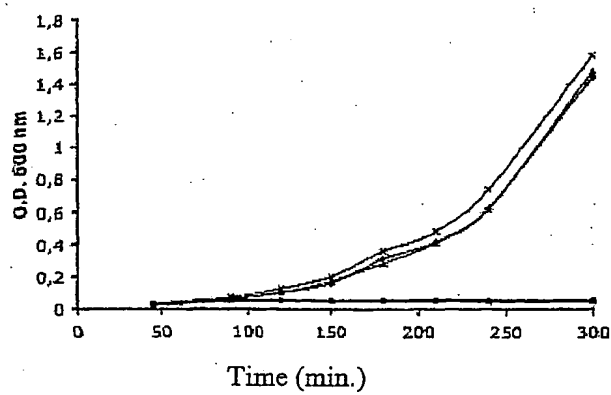


Figure 5A

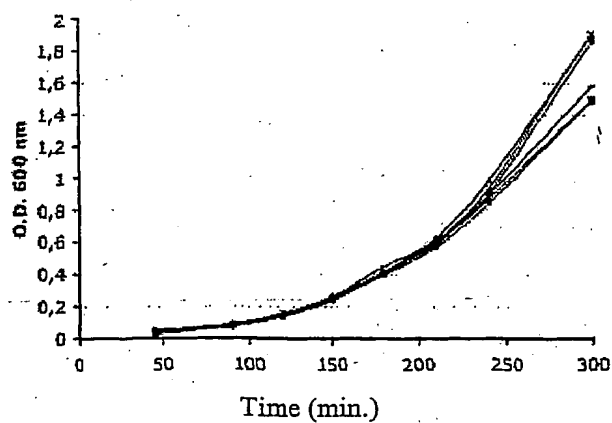


Figure 5B

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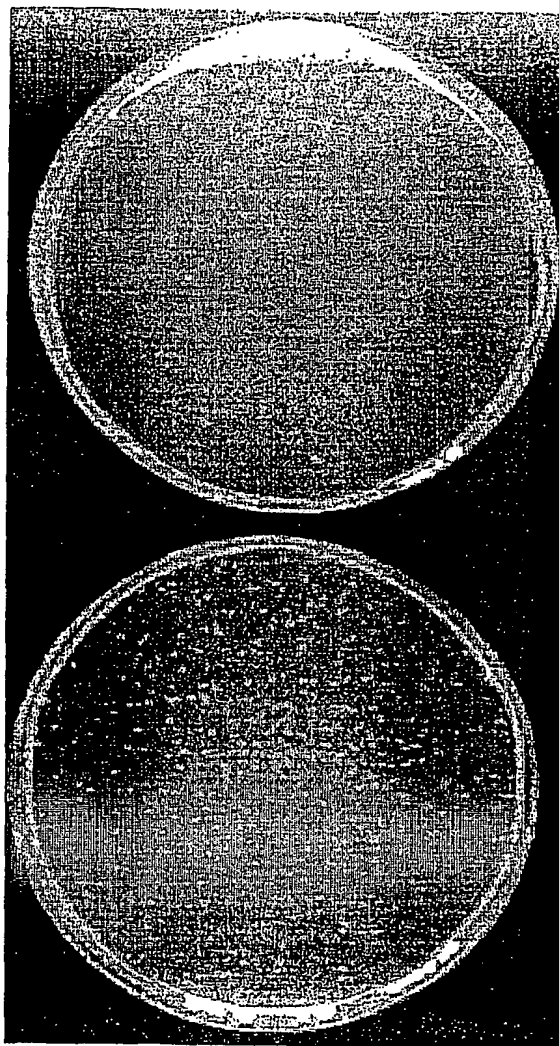


Figure 6

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